Automated iterative near-term

forecasting for the Portal Project

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12 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.
- 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.
- 41 Key-words: forecasting, prediction, mammals, iterative forecasting, Portal Project

42 Introduction

- Forecasting the future state of ecological systems is important for management,
- 44 conservation, and evaluation of how well models capture the processes governing
- ecological systems (Clark et al., 2001; Tallis & Kareiva, 2006; Díaz et al., 2015; Dietze,

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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.
   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
   progress of ecological forecasting and hindered our ability to make useful and reliable
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   predictions. The lack of active assessment results in limited information on how much
   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
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   longer a forecast remains out of date, the less accurate it becomes (Petchey et al., 2015;
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   Dietze et al., 2016). More regular updating and assessment will advance ecological
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   forecasting as a field by accelerating the identification of the best models for individual
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   forecasts and improving our understanding of how to best design forecasting
   approaches for ecology in general. For ecological forecasting to mature as a field, we
   need to change how we produce and interact with forecasts, creating a more dynamic
   interplay between model development, prediction generation, and incorporation of new
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   data and information (Dietze et al., 2016).
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   With the goal of making ecological forecasting more dynamic and responsive, Dietze et
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   al (2016) recently called for an increase in iterative near-term forecasting. Iterative
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   near-term forecasting is defined as making predictions for the near future and repeatedly
   updating those predictions through a cycle of evaluation, integration of new data, and
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   generation of new forecasts. Because forecasts are made 'near-term'—daily to annual
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   time scales instead of multi-decadal—predictions can be assessed more quickly and
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   frequently, leading to more rapid model improvements (Dietze et al., 2016; Tredennick
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   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
   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
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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
   mechanistic models can be compared to determine which model provides the best
   forecasts, thus providing insights into the importance of different ecological processes
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   (Dietze et al., 2016). Iterative near-term forecasting provides the more dynamic
   interplay between models, predictions, and data that has been identified as necessary for
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   improving ecological forecasting and our understanding of ecological systems more
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   broadly.
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   Because iterative near-term forecasting requires a dynamic integration of models,
   predictions, and data, Dietze et al (2016) highlight approaches to data management,
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   model construction and evaluation, and cyberinfrastructure that are necessary to
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   effectively implement this type of forecasting (Box 1). Data needs to be released
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   quickly under open licenses (Dietze et al., 2016; Vargas et al., 2017) and structured so
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   that it can be used easily by a variety of researchers and in multiple modeling
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   approaches (Borer, Seabloom, Jones, & Schildhauer, 2009; Strasser, Cook, Michener,
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   Budden, & Koskela, 2011). Models need to be able to deal with uncertainty, in both the
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   predictors and the predictions, to properly convey uncertainty in the resulting forecasts
   (Diniz-Filho et al., 2009). Multiple models should be developed, both to assess which
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   models are performing best (Dietze et al., 2016) and to facilitate combining models to
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   form ensemble predictions which tend to perform better than single models (Araujo &
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   New, 2007; Diniz-Filho et al., 2009). Ensuring that data and models are regularly
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   updated and new forecasts are made requires cyberinfrastructure to automate data
   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).
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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 10 to implement, and few of their recommendations are in widespread use in ecology today. 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 104 ecological study that collects high-frequency data on desert rodent abundances (J. 105 Brown, 1998; S. M. Ernest, Brown, Thibault, White, & Goheen, 2008). We constructed 106 an automated forecasting pipeline with the goal of being able to forecast rodent 107 abundances and evaluate our predictions on a monthly basis. In this paper, we discuss 108 our approach for creating this iterative near-term forecasting pipeline, the challenges we 109 encountered, the tools we used, and the lessons we learned so that others can create 110 their own iterative forecasting systems.

112 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) 114 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 118 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 122 with Sherman live traps for one night each month. For all rodents caught during a 123 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.

129 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 forms; in our case, this occurs monthly. Rebuilding models in an efficient and maintainable way relies on developing an automated pipeline to handle the six stages of converting raw data into new forecasts: data collection, data sharing, data manipulation, 134 modeling and forecasting, archiving, and presention of the forecasts (Figure 1a). To 135 implement the pipeline outlined in Figure 1a, we used a "continuous analysis" 136 framework (sensu Beaulieu-Jones & Greene, 2017) that automatically processes the 137 most up-to-date data, refits the models, makes new forecasts, archives the forecasts, and 138 updates a website with analysis of current and previous forecasts. In this section we 139 describe our approach to streamlining and automating the multiple components of the 140 forecasting pipeline and the tools and infrastructure we employed to execute each component. 142

143 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 individual components. Continuous analysis uses a set of tools originally designed for software development called "continuous integration" (CI). CI combines computing

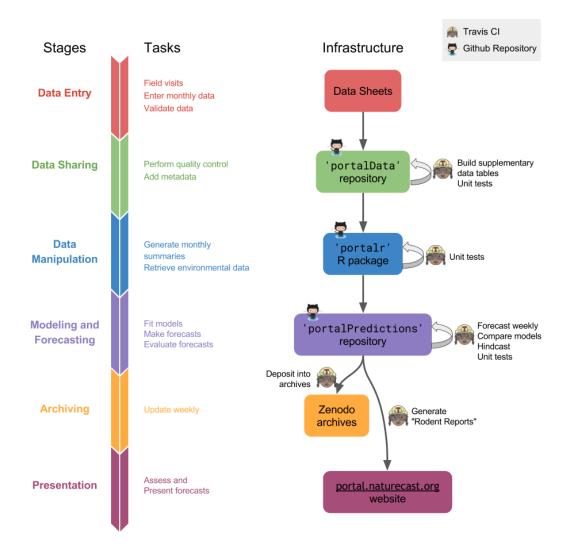


Figure 1: Figure 1. a) Stages of the forecasting pipeline. To go from raw data to forecast presentation involves a number of stages, each of which requires unique tasks, tools and infrastructure. The stages are interdependent, with outputs from one stage forming the inputs for the subsequent stage. Tasks 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).

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 150 change in the code or data, runs all the computer scripts needed to ensure that the forecasting pipeline runs from beginning to end. This is useful for iterative near-term 152 forecasting because it does not rely on humans to create new forecasts whenever new 153 models or data are added. These tools are common in the area of software development, 154 where they are used to automate software testing and integrate work by multiple 155 developers working on the same code base. However, these tools can be used for any 156 computational task that needs to be regularly repeated or run after changes to code or 157 data (Beaulieu-Jones & Greene, 2017). Our forecasting pipeline currently runs on a 158 publicly available continuous integration service (Travis CI; https://travis-ci.org/) that is 159 free for open source projects (up to a limited amount of computing time). Because of the 160 widespread use of CI in software development, alternative services that can run code on 161 local or cloud-based computational infrastructure also exist (Beaulieu-Jones & Greene, 162 2017). We use CI to quality check data, test code using "unit tests" (Wilson et al., 2014), 163 build models, make forecasts, and publicly present and archive the results (Figure 1b). 164 In addition to automatically running software pipelines, the other key component of 165 'continuous analysis' is making sure that the pipelines will continue to run even as 166 software dependencies change (Beaulieu-Jones & Greene, 2017). Many of us have 167 experienced the frustrations that can occur when software updates (e.g., changes in R 168 package versions) create errors in previously functional code. We experienced this issue 169 when the tscount package (Liboschik, Fokianos, & Fried, 2015), used by one of our 170 forecasting models, was temporarily removed from CRAN (the R package repository) 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) recommendation to use software containers. Software containers are standalone

packages that contain copies of everything needed to run a given piece of software, including the operating system. Once created, a software container is basically a time capsule, containing all the software dependencies in the exact state used to develop and run the software. If those dependencies change (or disappear) in the wider world, they still exist, unchanged, in the container. We use an existing platform, Docker (Merkel, 180 2014), to store an exact image of the complete software environment for running the 18 forecasts. Docker also allows a specified set of packages to be used consistently across 182 different computer and server environments. Using containers allows us to control 183 transitions to new package versions, implementing them only after we have tested them 184 and made any necessary changes to the data processing and analysis code. We use a 185 container created by the Rocker project, which is a Docker image with many important 186 R packages (i.e. tidyverse) pre-installed (Boettiger & Eddelbuettel, 2017). We add our 187 code and dependencies to this existing Rocker image to create a software container for 188 our forecasting pipeline. In combination, the automated running of the pipeline 189 (continuous integration) and the guarantee it will not stop working unexpectedly due to 190 software dependencies (via a software container) allows continuous analysis to serve as 191 the glue that connects all stages of the forecasting pipeline. 192

Data Collection, Entry, and Processing

Iterative forecasting benefits from frequently updated data so that state changes can be 194 quickly incorporated into new forecasts (Dietze et al., 2016). Both frequent data 195 collection and rapid processing are important for providing timely forecasts. Since we 196 collect data monthly, ensuring that the models have access to the newest data requires a 197 data latency period of less than 1 month from collection to availability for modeling. To 198 accomplish this, we automated components of the data processing and quality 199 assurance/quality control (QA/QC) process to reduce the time needed to add new data 200 to the database (Figure 1). 201

New data are double-entered into Microsoft Excel using the "data validation" feature. The two versions are then compared using an R script to control for errors in data entry. 203 Quality control (QC) checks using the testthat R package (Wickham, 2011) are run on the data to test for validity and consistency both within the new data and between the 205 new and archived data. The local use of the QC scripts to flag problematic data greatly 206 reduces the time spent error-checking and ensures that the quality of data is consistent. 207 The cleaned data are then uploaded to the GitHub-based PortalData repository (https://github.com/weecology/PortalData). GitHub (https://github.com/) is a software 209 development tool for managing computer code development, but we have also found it 210 useful for data management. On GitHub, changes to data can be tracked through the Git 211 version control system which logs all changes made to any files in the repository, giving 212 us a record of exactly of when specific lines of data were changed or added. All updates 213 to data are processed through "pull requests," which are notifications that someone has a 214 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 official version of the dataset. We also automated the updating of supplementary data tables, including information on 218 weather and trapping history, that were previously updated manually. As soon as new 219 field data is merged into the repository, continuous integration updates all 220 supplementary files. Weather data is automatically fetched from our cellular-connected 22 weather station, cleaned, and appended to the weather data table. Supplementary data 222 tables related to trapping history are updated based on the data added to the main data 223 tables. Using CI for this ensures that all supplementary data tables are always 224 up-to-date with the core data. 225

Data Sharing

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

236 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 238 manipulation but also a good understanding of the data to facilitate appropriate 239 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. 246 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 249 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
acquiring the data and handling common data cleaning and aggregation tasks. As a
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
package undergoes thorough automated unit testing to ensure that data manipulations
are achieving the desired results. Having data manipulation code maintained in a
separate package that focuses on consistently providing properly summarized forms of
the most recent data has made maintaining the forecasting code itself much more
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 models and make new forecasts each time the modeling code changes and when new data become available (Figure 1b). We use a plugin infrastructure to allow new models 265 to be easily added to the system. This approach treats each model as an interchangable black box; all models have access to the same input data and generate the same structure for model outputs (Figure 2). During each run of the forecasting code, all existing 268 models are run and the standardized outputs are combined into a single file to store the 269 results of the different models' forecasts. A weighted ensemble model is then added 270 with weights based on how well individual models fit the training data. This plugin 27 infrastructure makes it easy to add and compare very different types of models, from the 272 basic time-series approaches currently implemented to the more complex state-space 273 and machine learning models we hope to implement in the future. As long as a model 274 script can load the provided data and produce the appropriate output, it will be run and 275 its results incorporated into the rest of the forecasting system.

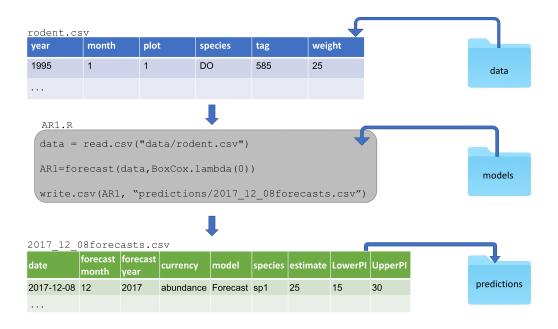


Figure 2: Figure 2. Demonstration of plugin infrastructure. All model scripts (represented here by the example AR1.R) are housed in a single folder. Each model script uses data provided by the core forecasting code (represented here by rodent.csv) and returns its forecast outputs in a predefined structure 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 28 this. Each forecast output file contains the date being forecast, the collection date of the 282 data used for fitting the models, the model name, the date the forecast was made, the 283 state variable being forecast (e.g., rodent biomass, the abundance of a species), and the 284 forecast value and associated uncertainty of that forecast (Figure 2). This allows us to 285 store a variety of different forecasts in a common format and may serve as a useful 286 starting point for developing a standard for storing ecological forecasts more generally. 287 Forecasts are currently evaluated using root mean square error (RMSE) to evaluate 288 point forecasts and coverage to evaluate uncertainty. We plan to add additional metrics 289 in the future. In addition to evaluating the actual forecasts, we also use hindcasting 290 (forecasting on already collected data; Jolliffe & Stephenson, 2003) to gain additional 291 insight into the methods that work best for forecasting this system. For example, a 292 model is fit using rodent observations up to June 2005, then used to make a forecast 12 293 months out to May 2006. The observations of that 12-month period can immediately be 294 used to evaluate the model. Since hindcasting is conducted using data that has already 295 been collected, it allows model comparisons to be conducted on large numbers of 296 hindcasts and provides insight into which models make the best forecasts without 297 needing to wait for new data to be collected (Harris, Taylor, & White, 2018). It can also 298 be used to quickly evaluate new models instead of waiting for an adequate amount of 299 data to accumulate. 300

301 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., 303 2016; Tredennick et al., 2016; Harris et al., 2018) (Figure 1). Archiving serves as a 304 form of pre-registration for model predictions because the forecasts cannot be modified 305 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 308 criterion means that GitHub is not sufficient for archival purposes because repositories 309 can be changed or deleted (Bergman, 2012; White, 2015). We explored three major 310 repositories for archiving forecasts: FigShare (https://figshare.com/), Zenodo 31 (https://zenodo.org/), and Open Science Framework (https://osf.io/). While all three 312 repositories allowed for easy manual submissions (i.e., a human uploading files after 313 each forecast), automating this process was substantially more difficult. Various 314 combinations of repositories, APIs (i.e., interfaces for automatically interacting with the 315 archiving websites), and associated R packages had issues with: 1) integrating 316 authorization with continuous integration; 2) automatically making archived files public; 317 3) adding new files to an existing location; or 4) automatically permanently archiving the files. Our eventual solution was to leverage the GitHub-Zenodo integration 319 (https://guides.github.com/activities/citable-code/) and automatically push forecasts to a 320 GitHub repository from the CI server and release them via the GitHub API. The 32 GitHub-Zenodo integration is designed to automatically create versioned archives of GitHub repositories. We created a repository for storing forecasts (https://github.com/weecology/forecasts) and linked this repository with Zenodo (a 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

automatically archives the resulting forecasts under a top-level DOI that refers to all
archived forecasts (https://doi.org/10.5281/zenodo.839580). Through this process, we
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
reproducible since the exact code used to generate every forecast is preserved. Early
forecasts from this system are archived in the modeling and forecasting code archive,
not in the newer repository 'forecasts'.

336 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 site (Figure 3; 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 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 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 archiving the forecast results.

48 Discussion

Following the recommendations of Dietze et al (2016), we developed an automated iterative forecasting system (Figure 1) to support repeated forecasting of an ecological system. Our forecasting system automatically acquires and processes the newest data,

Portal Forecast Total Abundance Forecast

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

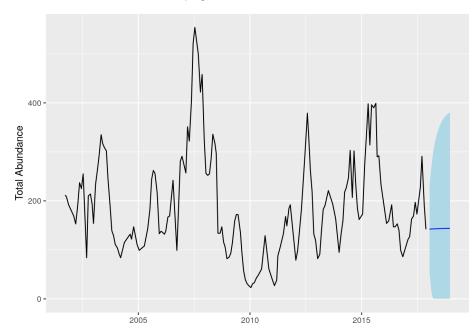


Figure 3: Figure 3. Screen capture of the homepage of the Portal Forecasting website (http://portal.naturecast.org). This site contains information on the most current forecasts, evaluation of forecast performance, and general information about the species being forecast.

refits the models, makes new forecasts, publicly archives those forecasts, and presents both the current forecast and information on how previous forecasts performed. Every 353 week, the forecasting system generates a new set of forecasts with no human intervention, except for the entry of new field data. Our forecasting system ensures that forecasts based on the most recent data are always available and is designed to allow 356 rapid assessment of the performance of multiple forecasting models for a number of 35 different states of the system, including the abundances of individual species and community-level variables such as total abundance. To create this iterative near-term 359 forecasting system, we used R to process data and conduct analyses and leveraged 360 existing tools and services (i.e. GitHub, Travis, Docker) for more complicated 361 cyberinfrastructure tasks. Thus, our approach to developing iterative near-term 362 forecasting infrastructure provides an example for how short-term ecological 363 forecasting systems can be developed. 364 We designed this forecasting system with the goal of making it relatively easy to build, 365 maintain, and extend. We used existing technology for both running the pipeline and 366 building individual components, which allowed us to build the system relatively cheaply 367 in terms of both time and money. This included the use of tools like Docker for 368 reproducibility, Travis CI continuous integration for automatically running the pipeline, 369 Rmarkdown and knitr for generating the website, and the already existing integration 370 between Github and Zenodo to archive the forecasts. By using this "continuous analysis" 37 approach (Beaulieu-Jones & Greene, 2017), where analyses are automatically rerun 372 when changes are made to data, models, or associated code, we have reduced the time 373 required by scientists to run and maintain the forecasting pipeline. To make the system 374 extensible so that new models could be easily incorporated, we used 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 2). 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 the performance of these forecasts can be assessed by both us and other researchers as new data is collected. This 380 serves as a form of pre-registration by providing a quantitative record of the forecast before the data being predicted were collected. While building this system was facilitated by the use of existing technological solutions, 383 there were still a number of challenges in making existing tools work for automated iterative forecasting. Continuous integration is designed primarily for running 385 automated tests on software, not for running a coordinated forecasting pipeline. As a 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 388 software package. In addition, hosted continuous integration solutions, like Travis, 389 provide only limited computational resources. As the number and complexity of the 390 models we fit has grown, we have had to continually invest effort in reducing our total 391 compute time so we can stay within these limits. Finally, we found no satisfactory 392 existing solution for archiving our results. All approaches we tried had limitations when 393 it came to automatically generating publicly-versioned archives of forecasts on a 394 repeated basis, and our eventual solution was difficult to configure to such a degree that 395 it will remain an impediment for most researchers. Overall, we found existing 396 technology to be sufficient to the task of creating an iterative forecasting pipeline, but it 397 required greater expertise and a greater investment of time than is ideal. Additional tool 398 development to reduce the effort required for scientists to set up their own short-term 399 forecasting systems would clearly be useful. Our efforts, however, show that it is 400 possible to use existing tools to develop initial iterative systems as a method for both 40 advancing scientific understanding and developing proof of concept forecasting systems. 402 Because of the breadth of expertise needed to set up our forecasting pipeline, our effort 403 required a team with diverse skills and perspectives, ranging from software 404 development to field site expertise. It is rare to find such breadth within a single 405

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 407 expertise, communication can be challenging (Winowiecki et al., 2011). We found a shared base of knowledge related to both the field research and fundamental 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 41 between field and computational/theoretical ecologists (http://weecology.org). Everyone on the team had received training in fundamental data management and computing 413 skills through a combination of university courses, Software and Data Carpentry 414 workshops (Teal et al., 2015), and informal lab training efforts. In addition, everyone 415 was broadly familiar with the study site and methods of data collection, and most team 416 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 418 interactions. Given the current state of tools for forecasting, forecasting teams will need people with significant experience in working with continuous integration and APIs. 420 This means interdisciplinary teams will generally be required for creating these 421 pipelines until tool development improves. To improve the success of these diverse 422 groups, we believe efforts at providing 'team science' training to scientists interested in 423 forecasting will be beneficial for the success of iterative forecasting attempts for the foreseeable future (Read et al., 2016). 425 We developed infrastructure for automatically making iterative forecasts with the goals 426 of making accurate forecasts for this well-studied system, learning what methods work 427 well for ecological forecasting more generally, and improving our understanding of the 428 processes driving ecological dynamics. The most obvious application of automated 429 iterative ecological forecasting is for speeding up development of forecasting models by using the most recent data available and by quickly iterating to 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 because new models can 43 quickly be applied to data and compared to existing models. The forecasting 438 infrastructure does the time-consuming work of data processing, data integration, and 439 model assessment, allowing new research to focus on the models being developed and 440 the inferences about the system that can be drawn from them (Dietze et al., 2016). We 441 plan to use this pipeline to drive future research into understanding the processes that 442 govern the dynamics of individual populations and the community as a whole. By 443 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 445 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 448 to forecast natural systems, understand the biology driving ecological dynamics, and 449 detect or even predict changes in system state that are important for conservation and 450 management.

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Data Accessibility

- The data used in this study is from the Portal Project and is openly available (CC0) on
- 462 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
- 465 (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
- 470 important.

471 Data

1. Frequent data collection

- 473 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).

486 Models

487 4. Focus on uncertainty

- 488 Understanding the uncertainty of forecasts is crucial to interpreting and understanding
- their utility. Models used for forecasting should be probabilistic to properly quantify
- 490 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 (Hooten & Hobbs, 2015).

5. Compare forecasts to simple baselines

- 494 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).

502 Cyberinfrastructure

- In addition to improvements in data and models, iterative near-term forecasting requires
- improved infrastructure and approaches to support continuous model development and
- 505 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 open licenses, good documentation, version
- control, and cross-platform support (Wilson et al., 2014; Hampton et al., 2015).

511 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.,
- 515 2016).

516 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).

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,
- ⁵²⁶ 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
- 529 community.

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