Closing the gap between statistical and scientific workflows for improved forecasts in ecology

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Abstract

Increasing biodiversity loss and climate change have led to greater demands for useful ecological models and forecasts. Relevant datasets to meet these demands have also increased in size and complexity, including in their geographical, temporal and phylogenetic scales. While new research often suggests that accounting for these complexities has a major impact on projected trends and forecasts, we argue that the typical approach to model fitting in ecology makes it impossible to evaluate and compare the models used to generate these insights and predictions. These problems stem in part from continuing gaps between statistical workflows—where the data processing and model development are often addressed separately from the ecological question and aim—and scientific workflows, where all steps are integrated. Yet, as ecologists become increasingly computational the opportunity to close this gap has never been greater. We outline how increased data simulation at multiple steps in the scientific workflow could revolutionize our understanding of ecological systems, yielding new insights for both trend estimation and forecasting. A shift toward universal training in a more robust model building could bridge the gap between process-based and statistical approaches and be transformative for ecological modeling.

Goal: Increase awareness of how we can merge statistical and scientific workflows in ecology (especially forecasting) and what we would get out of it.

1 Introduction

Anthropogenic drivers are reshaping natural systems (Díaz *et al.*, 2019). Impacts are projected to increase in coming decades, as climate change accelerates biodiversity loss, altering ecosystem services and human well-being (IPBES, 2019). Implementing sustainable policies to mitigate these impacts is thus a global priority, but designing the best policies requires estimating and understanding biodiversity and ecosystem trends to date alongside the skill to forecast future dynamics.

Meeting these policy needs has led often to two separate paths: one focused on estimating trends from new global datasets and another focused on forecasting from generally distinct datasets or mechanistic models based on less data. Newly available large-scale, long-term datasets have provided our first 'global' estimates of biodiversity trends (e.g. Loh *et al.*, 2005; Dornelas *et al.*, 2018), but these data—gathered opportunistically from multiple sources—are unbalanced with massive geographic, temporal and taxonomic biases. Models to date have failed to fully address these challenges and, perhaps because of these limitations, are rarely if ever used for forecasting. Instead forecasting—under different plausible scenarios—has generally relied on entirely different datasets combined with either correlative or process-based models (IPBES, 2019), with process-based models often promoted as the most realistic approach (Urban *et al.*, 2016; Pilowsky *et al.*, 2022) because they focus on mechanistic representations of ecosystem functioning. The current outcome from these approaches is no clear agreement on current species trends, with ongoing debates on the magnitude and even direction (Dornelas *et al.*, 2014; Leung *et al.*, 2020; Buschke *et al.*, 2021; Johnson *et al.*, 2024), and forecasts that diverge due to high model uncertainty at the ecological level (Cheaib *et al.*, 2012).

We argue that current debates and diverging forecasts are driven in large part by the incoherent and disconnected workflows used today in ecology (Loreau *et al.*, 2022; Talis & Lynch, 2023; Johnson *et al.*, 2024). Research estimating biodiversity trends has become focused on methodological aspects because the current workflow fails to examine the gap between ideal and available data, and rarely tests for predictive accuracy that could scale up to allow forecasting. At the same time, forecasting-focused process-based models often develop by adding new separate layers or components. These new parts are often disconnected from the original research aim, its data stream and the previous scientific insights, because current approaches rarely examine the model as a functioning whole and thus ignore major degeneracies.

Workflows that fully integrate all the steps required to build a model from an ecological question, evaluate its limitations and degeneracies, before estimating its parameters and making projections, could reduce many of these problems. In particular, we argue that workflows that incorporate data simulation at multiple steps can quickly identify flaws in model structure and constraints in data, and allow us to undertand when, where and why different models diverge. Towards this aim, we outline the steps of a universal workflow that could harmonize both trend estimation and forecasting.

2 Scientific method and workflows

Quantitative science relies on a model-based framework, to confront hypothesis with data (Chamberlin, 1965). In an idealized scientific method, we would formulate a research question and hypotheses, design an experiment accordingly, build a model, collect data, and using this data to inform our model and differentiate between hypotheses. But this idealized method often does not apply to the reality of ecological research, and most of macroecological insights emerge from exploring patterns in data. Many important questions cannot be addressed through controlled experiments and replications. Instead, we must often rely on existing, heterogeneous datasets alongside uncertain and incomplete theory to provide a large-scale and long-term perspective (Hilborn & Mangel, 1997).

This reality should drive researchers to use more robust and coherent methods, but the current workflows combined with the challenges ecologists are facing instead may lead to persistent problems. Trend estimation has focused mostly on fitting a model to empirical data in a uni-directional way that makes feedbacks to highlight uncertainty and related limitations in the model and/or data rare (Fig. 1). For forecasting, researchers have focused on making predictions with increasingly complex models, frequently obscuring the steps underlying model building and parameterization (Fig. 1). Today, researchers often calibrate different parts of the model separately, and fix some parameter values based on experiments and expert knowledge, to avoid problems when trying to fit the model as a whole. Addressing these problems while accounting for the realities of working with ecological data requires a more comprehensive workflow.

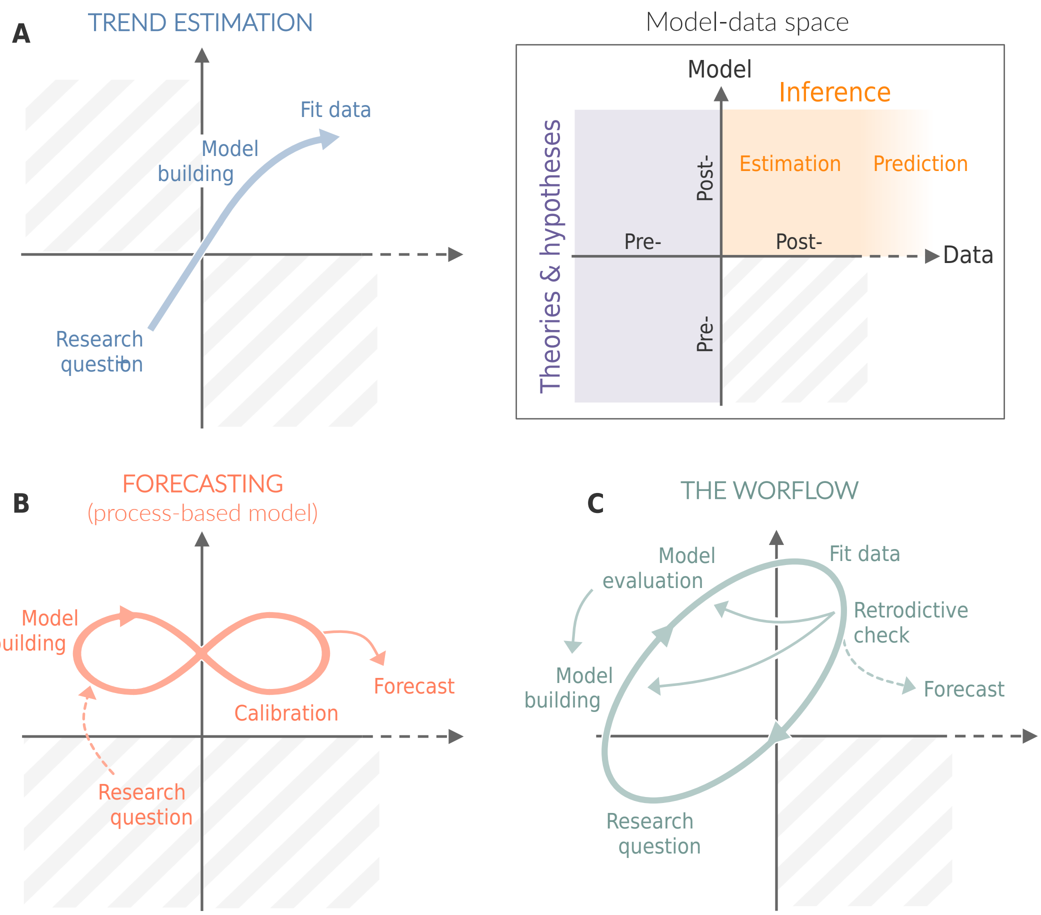


Figure 1: Here the caption could explain a bit more the pre-model pre-data to the post-model post-data...

We argue a workflow that moves along the data-model space in a coherent sequence of steps with repeated data simulation (Fig. 1c) could reduce many of these problems and thus improve ecological science. The first step of this workflow is to define an explicit research question and formulate hypotheses (Fig. 2). This involves making clear assumptions about the most influential drivers, within the specific context of our study. This step should guide the construction of a narrative model of how we believe the system works, focusing on the mechanisms that could generate the data we observe, including the observational error. From this narrative, we can then develop a mathematical model—an ensemble of equations that encapsulates our knowledge and is designed to answer our research question. The general idea is to start with a relatively simple model that we could refine later. At this stage, prioritizing biologically meaningful parameters is crucial, as it allows us to have a sense of plausible parameter values. This means choosing a model formulation where each parameter corresponds to an interpretable behavior (which sometimes requires to think about alternative parameterizations).

With a model in place the next step focuses on testing and understanding it via data simulation. 'Fake' or 'test' data are generated directly from the model by fixing parameters to some reasonable range of values (which is straightforward if the parameters are interpretable) and from fake predictor data (Fig. 2). This simulated data should reflect the full model assumptions, and could begin to include complexities in our data structure and biases, which may in turn lead to adjusting the model. For example, if a researcher realizes their empirical data is geographically biased, then this bias should be built into the model and thus then into this data simulation step. We then fit our model to this simulated dataset and evaluate its ability to recover the prescribed values.

Once we are confident about our model structure, we can introduce real data as part of an initial model fitting step. This way, we obtain parameter estimates constrained by observations. Here, difficulty in fitting the model might indicate an inherent need for more data to address our initial question, or re-evaluate the model of how we think the system works. This could lead us to either simplify our research question or—ideally—launch new data collection efforts. This leads to the second data simulation step, this time using our fitted model parameters to generate predictions. This retrodictive check allows model output to be compared to observations. The workflow encourages a focus on the full model, and replaces parameters at the core of the modeling process, as fundamental components that shape both inference and forecasting. Any parameter (such as a trend estimate) must be carefully interpreted alongside others. Within such a workflow, forecasting emerges as a natural outcome: rather than being a final goal, it only involves jointly modeling new circumstances along with the original data.

A key feature of this workflow is the central role of data simulation, which introduces two feedback loops. The first feedback arises when we evaluate the model on simulated data. The failure of the model to recover known parameter values and handle the complexity of the simulated data should prompt a reconsideration of the model, or even a reformulation of the research question. Further, this step might reveal that some parameters are highly non-identifiable, flagging the need to change the model structure—before incorporating real observations. The second feedback loop comes from the retrodictive check. Discrepancies may indicate a missing key driver—perhaps an expected outcome if we known our initial model was too simplistic. We can refine the model to integrate the missing process and restart the workflow. Insights from the retrodictive check can also lead us to introduce additional complexity when simulating fake data, such as phylogenetic structure or observational biases (e.g. unbalanced data). This iterative evaluation of the model moves beyond a simple reliance on goodness-of-fit metrics. At each iteration, we are able to evaluate the model behavior, both with simulated and real data, taking into account our expert knowledge of the ecological processes.

3 The workflow in practice

Across the different fields of ecology—for both parameter estimation and forecasting—a systematic application of a coherent workflow could highlight the best opportunities to reduce uncertainties

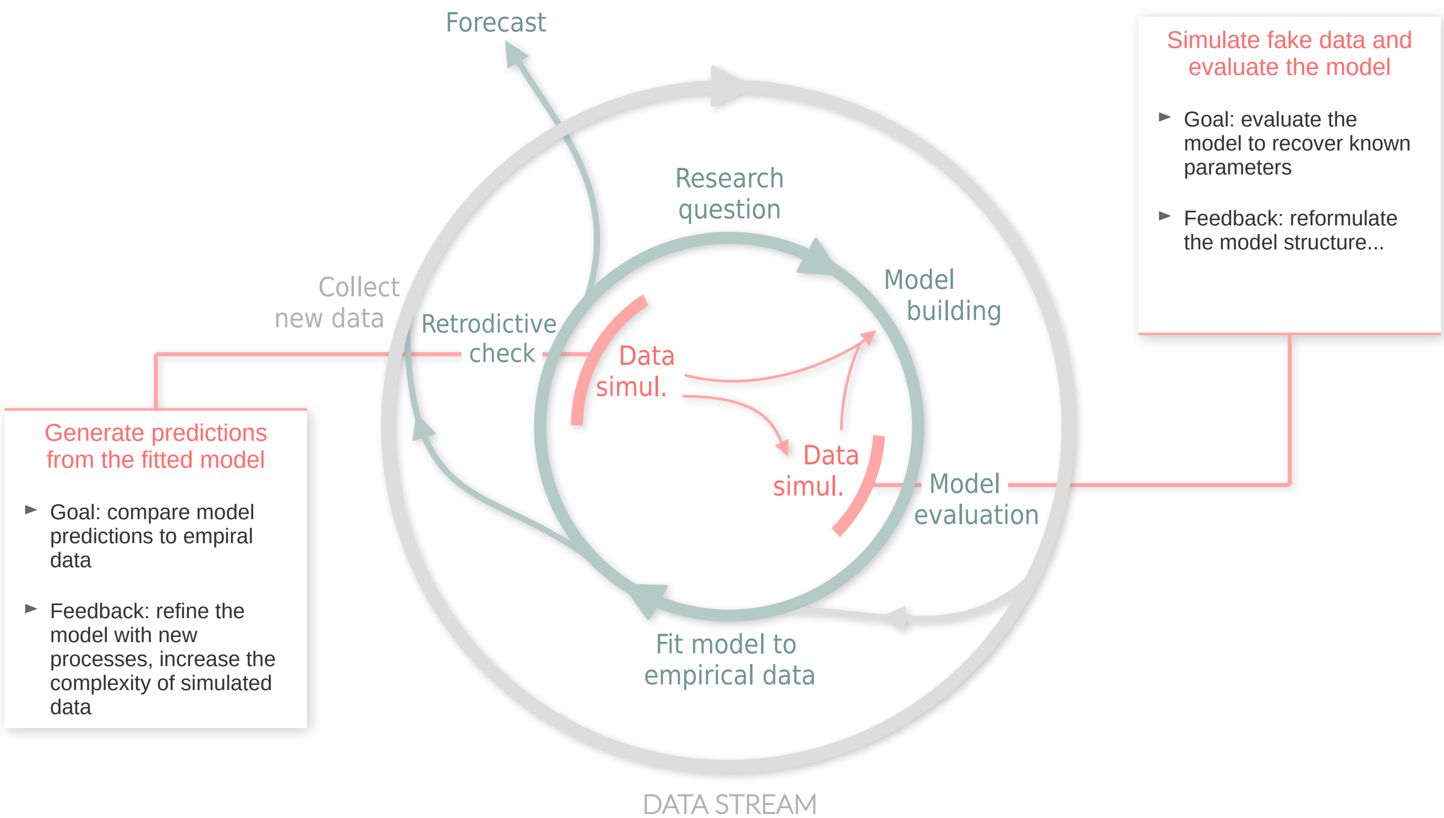


Figure 2: Here we could have a caption like ... Our workflow builds on others (with citations) to highlight the integrated nature of stuff in ecology. We can work on this once we get feedback from mighty co-authors. Also, should we list the steps on the figure? What do people think?

through new scientific insights, toward the most critical steps. This will help refocus the debate on designing new hypothesis, formulating new questions—and guiding efforts to collect new data. Here, we illustrate how such a workflow could lead to significant improvements in two case studies: (i) estimating global biodiversity trends and (ii) forecasting future species and ecosystem dynamics using process-based models.

3.1 Trends

Ecologists today have amassed data on populations and species across the globe; they have also engaged in an increasing number of debates on regional and global trends, with arguments over the magnitude and even direction of population and biodiversity metrics (Dornelas *et al.*, 2014; Leung *et al.*, 2020; Terry *et al.*, 2022; Müller *et al.*, 2024). While shifting estimates are part of the process of science—refining our approaches and thus estimates over time—we believe these debates would be much reduced and more rapidly resolved through use of an improved workflow.

An improved workflow that required data simulation and retrodictive checks would lead to larger model advances and a greater recognition of uncertainty—thus highlighting likely consistency in estimates across models—that could better aid policy. Using the workflow would make what now appear as major discrepancies more obviously shifts in point estimates that are generally all in the same uncertainty space (Johnson *et al.*, 2024)—and it would challenge modelers to show major predictive advances, which is not currently part of the process. Explanatory power in most models of observational data is usually very low (Low-Décarie *et al.*, 2014; Møller & Jennions, 2002) and thus tests of models' predictions rarely expected. But the workflow highlights that predictions from the model—what we call retrodictive checks—are part of the process of science, and critical to testing for what may be missing in a model. We expect retrodictive checks on most published trend analyses would highlight major missing components in these models, and drive changes both in the models themselves and in the simulated data to check the models. While ecologists have started to use simulated data more to understand potential limitations of their models and data combined, this is still extremely rare, and efforts to date often treat simulations as separate from the statistical model (Buschke *et al.*, 2021; Dove *et al.*, 2023), short-circuiting their full utility.

Applying the workflow to current trend estimates could importantly highlight the best way to improve data collection for more reliable estimates. Returning to the example of a global estimate of trends in vertebrate populations of species over time and applying our proposed workflow would mean more efforts to define the goal and question—is it a simple global estimate? Or a need to also find which species are declining most, including those that may have poor or no data? From there a generative model using simulated data for testing could incorporate many aspects of the populations, and data, that are often only included in 'null' or 'synthetic data generation' currently (Buschke *et al.*, 2021; McRae *et al.*, 2025) but could be built into the models fit to the empirical data. Eventually fitting the empirical data and performing retrodictive checks would likely highlight major missing components of the generative model and, ultimately, this would help inform our global estimates of mean trends. For example, certain populations are recovering for very specific reasons (e.g., elephants in regions where the ivory trade drove declines in the past) that perhaps should be modeled. From this model, what data are most critically needed to address the updated aims would become clearer and could drive new data collection (Toszogyova *et al.*, 2024).

3.2 Forecasting

Ecological forecasting is a broad field with a diverse range of methods. Process-based modeling is often considered the gold standard in ecology (Urban *et al.*, 2016; Pilowsky *et al.*, 2022) and beyond. Newer models generally incorporate greater complexity and an ever-growing number of parameters, making it more difficult to increase scientific understanding (Franklin *et al.*, 2020), and suggest or model potential policies.

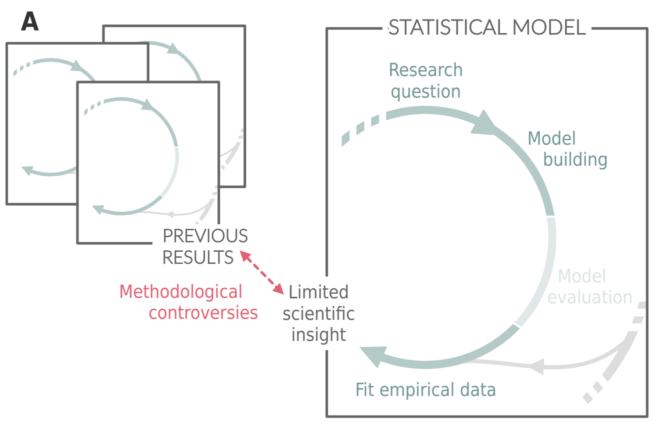
Increasing model complexity can be beneficial, especially when it reduces uncertainty; however, this is not always the outcome. In climate modeling, the uncertainty range on the effect of increasing CO_2 concentration on temperature have remained largely unchanged (Zelinka *et al.*, 2020). This has driven calls for more rigorous and transparent calibration processes (Balaji *et al.*, 2022). Similar concerns arise in ecology, where strong disagreements exist about the effect of climate change on future species distributions (Cheaib *et al.*, 2012) and ecosystem dynamics (Lovenduski & Bonan, 2017). These uncertainties have large implications beyond ecology, as they influence simulations of biosphere-atmosphere interactions and, ultimately, future climate projections (Bonan & Doney, 2018; Simpson *et al.*, 2025). Some researchers now advocate for the simplification of models, to avoid over-parametrization when the data provide little information to constrain some parameters (Wang *et al.*, 2017; Harrison *et al.*, 2021). If a model becomes too complex, understanding the sources of uncertainty and how they propagate through the model may become nearly impossible. Each additional process and parameter can increase overall uncertainty to the point where model projections lose their usefulness for decision makers (Saltelli *et al.*, 2020).

Applying the workflow to process-based models would help open the black box. Each successive step of model development in the workflow may highlight current problems and a path to solutions. Incorporating data simulation would introduce a crucial step between model building and data fitting, ensuring a clear delineation between the two and help expose potential degeneracies in the model design. Uncovering degeneracies would likely force researchers to begin with a simpler version of the model, which they could build on iteratively, testing for support—or lack thereof—when adding model complexity. The workflow may also highlight degeneracies by requiring more explicit model calibration, which is currently hidden within opaque 'model building', making it easy to hide non-identifiability in the model (where certain parameters cannot be uniquely estimated). Through the workflow non-identifiable parts of models could be addressed by reformulating the mathematical structure of certain processes, or finding ways to apply additional constraints (e.g., narrower ranges for certain parameters or developing new hypotheses that target the appropriate level of complexity). The resulting process-based models would likely be simpler and thus more tractable for quantifying parameter uncertainty and propagating it through projections.

Beyond improving the model building, the workflow also has the potential to shift how process-based models are perceived, particularly by those unfamiliar with them. The workflow could refocus attention on the research question, highlighting the ecological hypotheses that justify the use and design of the model. It would thus define a clear and limited context in which the model should apply, without always arguing about the necessity of adding more and more complexity. Process-based model would once again be a way to answer a research question—whereas today, model simulations have increasingly become a subject of study on their own. Ideally, applying the workflow would help to move away from the traditional process-based model paradigm, where parameters are typically assigned fixed values without properly accounting for their uncertainty. Instead, it would guide a step-by-step model fitting, parameter estimation, and uncertainty quantification.

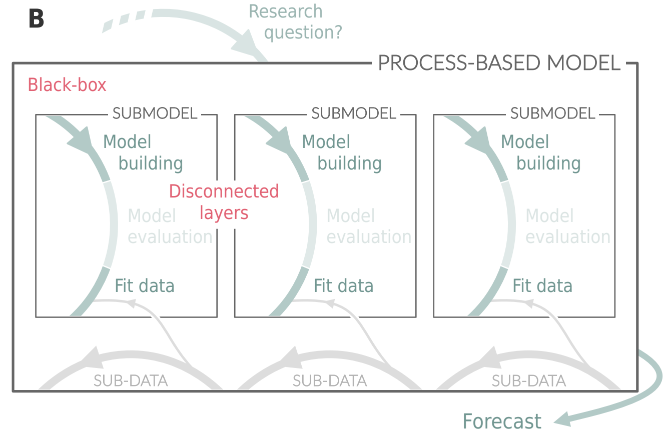
This shift would present a significant challenge—as it would likely reveal many issues related to model degeneracies and data limitations before achieving robust inference. But ultimately, it would prevent modelers from making biased inferences and unfounded assumptions beyond what the data can support.

Trend estimation



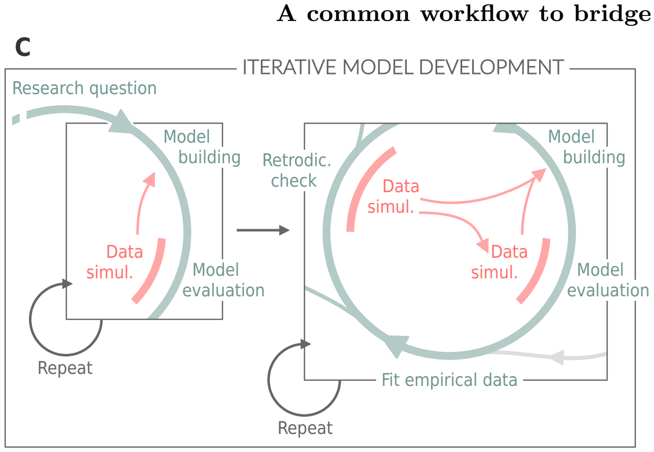
In the current workflow for estimating trends over time a new model with a new estimate often leads to a paper (see Fig.) because ecologists spend far too little time interrogating their models with simulated data, or their model performance fit to empirical data. The Living Planet Index (LPI), which aims to include long-term data on vertebrate populations of species across the globe is emblematic of these conflicting results. With updated data released semi-annually (??) alongside new estimates of decline, a growing number of high-profile papers have challenged how strong the evidence is for population decline (Dornelas *et al.*, 2014; Gonzalez *et al.*, 2016; Wagner *et al.*, 2021; Müller *et al.*, 2024), with each paper taking a slightly different analytical approach. For example, Leung *et al.* (2020) published a mixture model that suggested most populations were not significantly declining, followed by other alternative modeling approaches (Buschke *et al.*, 2021; Puurtinen *et al.*, 2022) including a recent one suggesting a basic analysis of the dataset should always include three sources of autocorrelation, finding trends that encompassed most previous results (Johnson *et al.*, 2024).

Mechanistic forecasting



Model development is the central step of the process-based workflow, typically requiring several years, yet it often remains opaque from an external perspective. The step of designing the model—translating knowledge and hypotheses into mathematical equations and parameters—is often blurred with the step of model calibration (or tuning), where parameter values are inferred. Models are often treated as an accumulation of multiple submodels, each governing one or several ecological processes. Rather than being fitted as a whole, submodels are calibrated separately against specific subsets of data, and some parameters are simply prescribed (i.e. fix to a value found in the literature) or tuned to reproduce some observations or theory. The way models are currently calibrated is not a coincidence, but rather an inappropriate way to accommodate their complexity, where many parameters compensate for one another.

A common workflow to bridge trend estimation and forecasting



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An universal workflow offers an opportunity to bridge statistical and process-based frameworks, integrating mechanistic knowledge and leveraging robust statistical approaches (e.g. Rounce *et al.*, 2020). Process-based models would no longer be perceived as deterministic black boxes by other researchers but rather as robust statistical frameworks encapsulating both data structure and mechanistic knowledge. And it would also be an opportunity to spread the incorporation of mechanistic assumptions beyond the process-based modeling community.

4 Barriers and opportunities

We believe our workflow could help advance ecological science and its applications, but widespread use of it requires overcoming major hurdles that pervade science. One well-known hurdle is the pressure to publish, which can lower research standards and make the added effort of this workflow seem ill-placed. This may be especially true for those who see science rewarded mostly through the shear number of publications. But for those more focused on the long-term value of their work—for example, how well cited their papers are over a longer-time scale—we think this workflow can help. Further, growing concerns about how reproducible science is, especially in ecology where samples sizes are low and effects likely non-linear and complex, we believe adopting the workflow will pay off in the longer term, as more value is placed on research that carefully developed, openly shared (for data and code) and acknowledges its uncertainty towards the aim of improving future data collection and model development (see Fig).

4.1 Adopting the workflow

Advancing ecology to where most researchers use models built more flexibly from ecological theory and insights applied to their ecological systems will not happen rapidly without a major shift in training. Much of ecology still divides the world into training for those focused on several groups: those who gather data and learn a limited set of pre-built models versus those who develop more complex models. In ecological training today researchers who conduct field and lab studies often learn a highly limited set of particular tests matched to particular experiment designs and simple information on their variable types (e.g., categorical x and y leads to using a chi square test). Such training leaves a large number of ecologists adrift later when asked to simulate any sort of simple model because they were never taught what a model fundamentally is.

Instead, ecologists trained in a limited set of tests are expected to collaborate with others when they need more complex models, who were trained more in model development (though often for highly specific applications, such as wildlife population estimates, where they may rarely develop entirely new generative models). These two groups further differ from process-based modelers, who often train in physical and ecophysiological processes and how to abstract them into mainly deterministic models. Few of these groups have integrated data simulation into their statistical or scientific workflows, which is generally reserved as a form of training needed mainly by those specializing in theoretical ecology, who often solve analytical equations but rarely link to empirical data. While specialization is valuable, we argue the fundamental training in ecology has overly-siloed these groups and prevented more rapid progress.

Training all ecologists in our proposed workflow would break down barriers between these different groups with likely major benefits for science. Instead of training some ecologists extensively in experimental design and tests that may match certain designs (though rarely do for ecological data, CITES), training in our workflow would focus on learning to generate questions and then models, and then to simulate data from them. This would mean training all ecologists to link the ecological processes they study with the mathematical models that may describe them. Through this and retrodictive checks most ecologists would more easily think through what parameters are most critical to their question and or aim (e.g., management) and also gain a much stronger connection to the level of uncertainty in many of ecological estimates. Empirical ecologists would be more likely to recognize critical gaps in current models fit by those specializing in ecological modeling and help advance those models. Process-based modelers may start a new generation of simpler models that are more tractable to theoretical ecologists, who may suddenly see bridges from their work to empirical data and forecasting. Those focused on learning complex statistical models may find many of the field now share their excitement and interest in more generative models, and could focus on adapting approaches to better forecasts or something.

4.2 A tractable alternative to machine learning

In a world where machine learning is rapidly advancing, there is no point of sticking to traditional methods if no changes are made. Machine learning will likely surpass process-based models if the latter lack a robust estimation of their parameters and fall in a complexity trap, at the cost of their interpretability. Similarly, trend analysis, when the focus is on methodological controversies (due to the lack of an iterative workflow) rather than on a robust mechanistic foundation, offers no clear advantage over machine learning.

Today model development in ecology is rarely transparent, which limits how easily the research community can understand modes, and thus identify potential issues. Instead of broad inclusive conversations about how to improve models to advance our ecological understanding, a significant portion of scientific debate today has become lost in methodological considerations, but we believe our workflow provides an tractable step to fixing this. By focusing on model development more tightly tied to ecological expertise, we ague this workflow should broader the community that contributes to model development. As ecologists are increasingly expanding their computational toolkits, many field, and lab and other forms of 'empirical' ecologists have the basic tools to follow this workflow to build models that better represent their ecological, and—most importantly—to interrogate them.

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