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A Toolkit for Ecosystem Ecologists in the Time of Big Science

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Abstract

Ecosystem ecologists are being challenged to address the increasingly complex problems that comprise Big Science. These problems include multiple levels of biological organization that cross multiple interacting temporal and spatial scales, from individual plants, animals, and microbes to landscapes, continents, and the globe. As technology improves, the availability of data, derived data products, and information to address these complex problems are increasing at finer and coarser scales of resolution, and legacy, dark data are brought to light. Data analytics are improving as big data increase in importance in other fields that are improving access to these data. New data sources (crowdsourcing, social media) and ease of communication and collaboration among ecosystem ecologists and other disciplines are increasingly possible via the internet. It is increasingly important that ecosystem ecologists be able to communicate their findings, and to translate their concepts and findings into concrete bits of information that a general public can understand. Traditional approaches that portray ecosystem sciences as a dichotomy between empirical research and theoretical research will keep the field from fully contributing to the complexity of global change questions, and will keep ecosystem ecologists from taking full advantage of the data and technology available. Building on previous research, we describe a more forward-looking, integrated empirical–theoretical modeling approach that is iterative with learning to take advantage of the elements of Big Science. We suggest that training ecosystem ecologists in this integrated approach will be critical to addressing complex Earth system science questions, now and in the future.

Key words: multiple levels of organization; interacting spatial and temporal scales; technological Advances; big data; analytics; crowdsourcing; machine learning.

Ecosystem ecologists are being challenged to address increasingly complex problems as knowledge about the Earth as a coupled system of land–water–atmosphere interactions and feedbacks increases (Foley and others 2003; Julian and others 2008; Peters and others 2008; Treasure and others 2015). These problems include multiple levels of biological organization (from individual plants, animals, and microbes to populations and communities within ecosystems) that cross multiple interacting temporal and spatial scales, from individuals to landscapes, continents, and the globe (for example, Carney and Matson 2005; Schmitz and others

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2014; Peters and others 2007, 2014b; Preston and others 2016). As technology improves and new technology is developed, the availability of data, derived data products, and information to address these complex problems are increasing at finer and coarser scales of resolution, and legacy dark data are being brought to light (for example, Collins and others 2016; Kim et al. 2016;Zinnert and others 2016). Data analytics are improving as big data increase in importance in other fields that are improving access to these data, and a machine learning process is being developed to improve scientific community efficiency through time (Peters and others 2014a). New data sources (for example, citizen science, crowd sourcing, social media) and ease of communication and collaboration among ecosystems ecologists and other disciplines are increasingly possible via the internet (Aceves-Bueno and others 2015; Silberzahn and Uhlmann 2015). As the complexity of the ideas and the amount of data increase, it will become increasingly challenging, yet even more important, that ecosystem ecologists be able to communicate their findings, and to translate their concepts and findings into concrete bits of information that a general public can understand (Oreskes and Conway 2010).

All of these elements (complex questions that include multiple levels of organization and interacting spatial and temporal scales, new and improved technology, big data analytics and machine learning, new data sources, communication and collaboration opportunities, translation to the public) constitute issues associated with Big Science, and due to the nature of the discipline, ecosystem ecologists are at the nexus of these issues. Here, we contend that the traditional view of ecosystem ecology, where an empirical approach is distinguished from a theoretical approach, will be insufficient in the time of Big Science. Furthermore, this distinction will keep the field of ecosystem ecology from fully contributing to the complexity of global change issues, and will keep ecosystem ecologists from taking full advantage of the big data and advances in technology becoming available.

We start by briefly describing the traditional approaches to addressing questions in ecosystem ecology with a focus on their differences, and then we describe a more forward-looking, integrated, and iterative approach with learning that takes advantage of the elements of Big Science. We provide support for our ideas by citing numerous papers from the *Ecosystems* journal to illustrate the breadth and diversity of topics covered by ecosystem ecologists.

Traditional Approaches to Ecosystem Science

In the traditional approaches to conducting ecosystem science, there is a dichotomy between empirical and theoretical approaches. We recognize that ecosystem ecologists may use a combination of these approaches, but here we describe the end members to provide a clear distinction between them. We differentiate these two approaches based on the realm of inference and focal ecosystem or geographic location of the research question (sensu Peters and others 2012), and recognize there may be other ways to distinguish between them. In our dichotomy, process-based numerical models and analytical methods can be part of the toolkit in both approaches.

In a Traditional Empirical Approach

scientists are interested in addressing research questions that explain patterns and dynamics that are site-specific (that is, for specific geographic locations, ecosystems, or targeted areas), where observations and data can be collected and specific questions have particular relevance. An example of this work is the study by Chen and others (2016) who examined effects of changes in climate on energy and water budgets on a particular savanna-woodland ecosystem using a combination of empirical observations and a detailed mechanistic model. In such an approach, scientists start with observations and intuition, including past experience from the site or location, to develop a mental model of the system and an approach to the problem to be addressed (Fig. 1A). Building on knowledge from the literature and discussions with colleagues, a conceptual model for the problem, that includes the components of the ecosystem and their relationships to each other and to their environment, is developed. Hypotheses or questions are then generated and are tested using field and laboratory data that are collected by that individual researcher or their group. These data can be supplemented with ancillary open-source information, such as climate and soils data. Often this information needs to be transformed through aggregation and standardization procedures before it can be used. A researcher can use this information to either test hypotheses using analytical methods or to address specific questions by

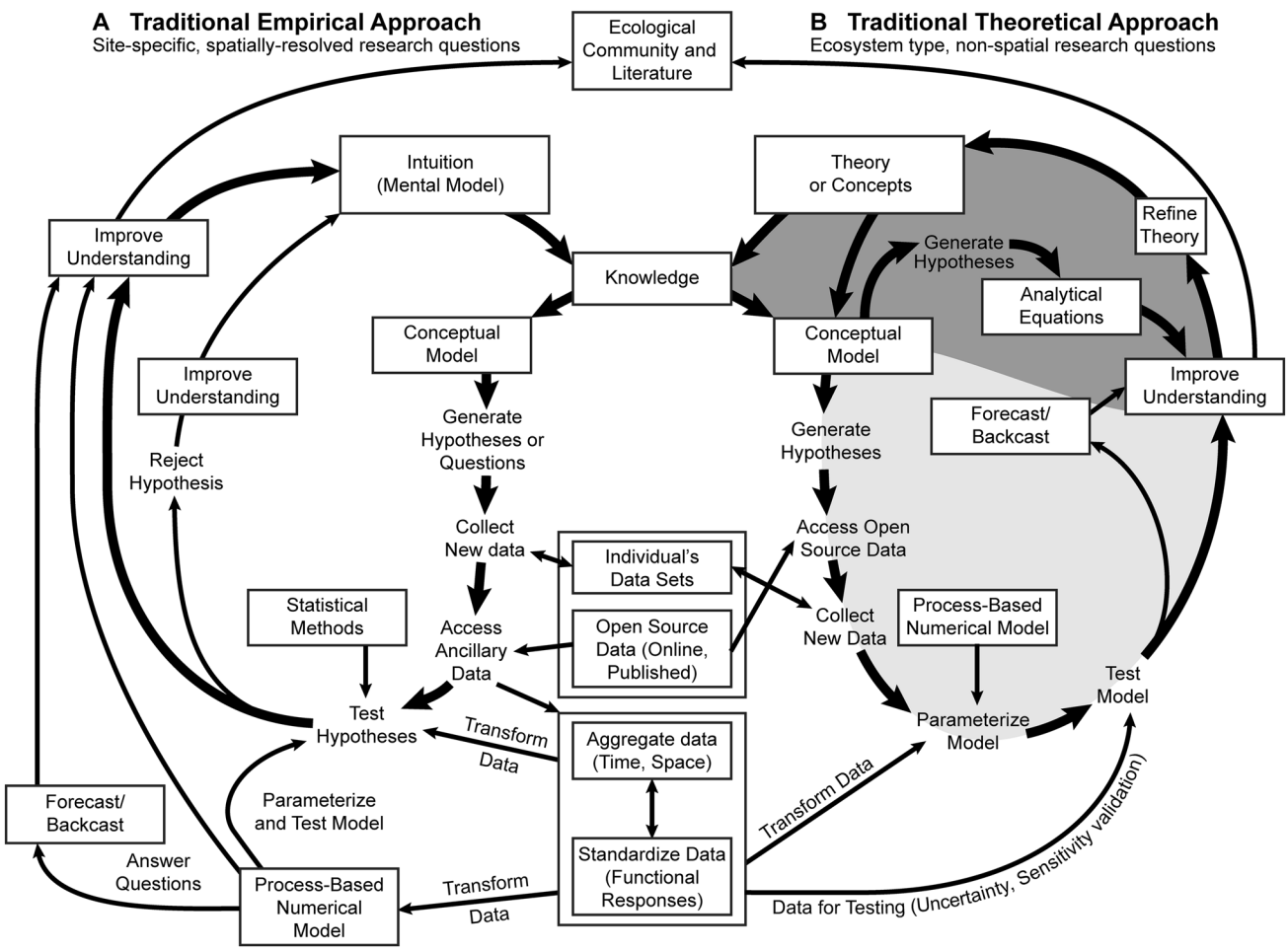
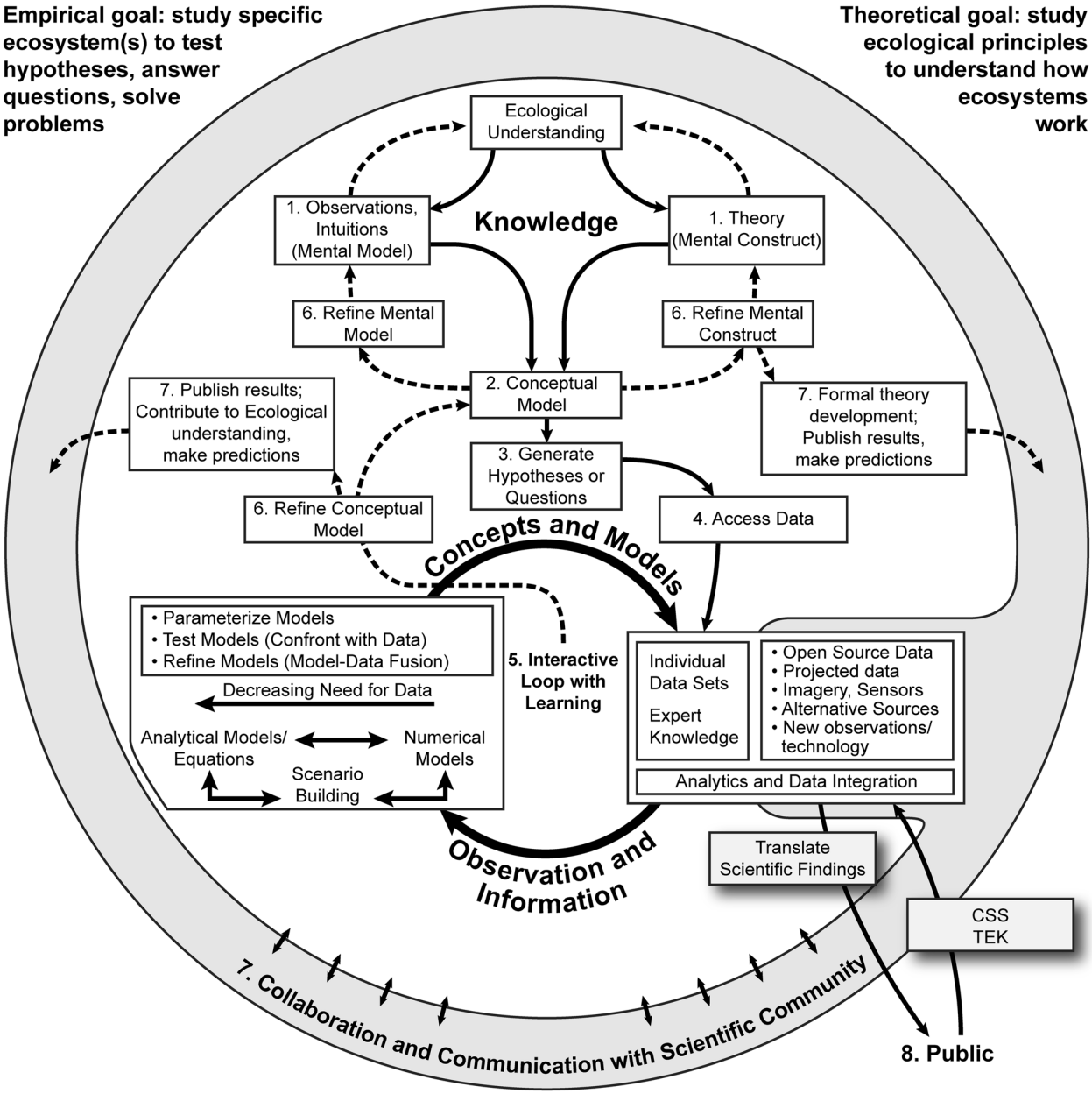


Figure 1. Traditional approaches to ecosystem science: A. Empirical approach focuses on site- or ecosystem-specific questions that are spatially resolved; B. Theoretical approach focuses on general ecological principles for ecosystem types that are not necessarily located in spatially resolved geographic locations. Figure expands upon ideas presented in Peters and others (2014a) for a hypothesis-driven scientific approach.

parameterizing, testing, and running experimental simulations with a numerical model. For hypothesis testing, regardless of whether the hypotheses are rejected or accepted, there is improved understanding about the ecosystem for the individual researcher that leads to an improved or refined mental model. Publication of the results leads to improved understanding among the broader ecological community interested in this ecosystem or in ecosystems with similar processes, organisms, or dynamics.

For answering specific questions under the traditional empirical approach, a researcher's data, in combination with ancillary information, can be used to parameterize and test numerical models that are developed based on relationships in the conceptual model. Tested models can be used to: (a) create forecasts of future ecosystem dynamics under alternative climatic, atmospheric, or management conditions expected at that research site; (b) create backcasts of historic ecosystem dynamics under previous climatic, atmospheric, or management conditions at that research site; and (c) improve understanding about ecosystem behavior. Regardless of the specific goal, improved understanding for the ecological community results through the publication of research findings. This empirical approach that integrates data and process-based modeling in an iterative way through time to improve understanding about specific research sites with extensions to the ecosystem type is reflected by research conducted at NSF-supported Long Term Ecological Research sites (for example, Groffman and others 2012; Peters and others 2015). This improved understanding often leads to new questions.



In a Traditional Theoretical Approach

Scientists are interested in research questions that are generally applicable based on ecological principles, and not geographically location-specific (Figure 1B). In this approach, a scientist starts with a theory or a set of concepts. These ideas are further developed with knowledge from the literature or discussions with colleagues into a conceptual model showing relationships among the components. At this point, a purely theoretical approach diverges from a numerical modeling approach. A purely theoretical approach provides a framework of concepts and propositions that generates testable hypotheses (for example, Allen and others 2014). These hypotheses may be tested using analytical models, often as a set of differential equations, which represent a subset of processes occurring in ecosystems (Figure 1B, dark-shaded area). Adding additional concepts can refine the theory and generate new ideas for testing. Theoretical models contain only highly idealized representations of a small number of processes and drivers; thus, they are not intended to represent real ecosystems, but rather are useful in elucidating

◀ **Figure 2.** An integrated empirical–theoretical modeling approach that is iterative with learning. For any given question, an individual scientist will enter the process either with a goal to study a specific ecosystem or location(s) to answer questions and test hypotheses about the dynamics of these ecosystems, or with a goal to understand how ecosystems function using basic principles. In either case, a mental model based on observations or mental construct based on theory will be the first *step* followed by access to the ecological knowledge base to assist in building a conceptual model as to how the system works (*step* 2) and generating testable hypotheses or questions (*step* 3). The scientist then accesses data and information from multiple sources that are relevant to the hypotheses or questions (*step* 4), and enters the concepts + data + modeling iterative loop with learning (*step* 5). Additional experiments may be conducted, and online data may be obtained from open sources or protected data that require special handling. Increasingly new sources of information are becoming available, including from crowdsourcing and citizen science networks (CSS), traditional ecological knowledge (TEK), and derived data or modeling products from sensors and imagery. Data integration and mashups will be required before statistical analyses can be conducted. The data can be used to parameterize and test the various analytical, numerical, and scenario models that are increasingly becoming available to ecologists. After going around the loop a sufficient number of times, learning each time around and refining the conceptual model (similar to machine learning [Peters and others 2014a]), the researcher will have a refined mental model (*step* 6), will be ready to generate publishable products for the scientific community (*step* 7), and translate their scientific findings to a non-scientific audience (*step* 8).

general principles, or new behaviors of a system. For example, the models of Rietkerk and others (2004) are useful for understanding and comparing patterns among ecosystem types. Concepts derived through this theoretical approach have been used to guide land management practices, even without formal hypothesis testing (for example, Lockwood and Lockwood 1993; Briske and others 2010). However, these concepts often have limited applicability to real world problems. Nonetheless, they are useful in terms of our abstract understanding of ecological system dynamics.

A numerical modeling approach also starts with concepts derived from a theory that lead to the development of a conceptual model and generation of hypotheses about ecosystem behavior under alternative drivers or management scenarios. The next step is to obtain published data and online information (that may be standardized and/or transformed) along, perhaps, with the strategic collection of new data to develop and parameterize a process-based, numerical model. This model is typically a system of differential equations that represents the states, processes, and driving variables of interest in the ecosystem (Figure 1B, light shaded area). The degree to which data are used to parameterize and test a model determines if a theoretical ecosystem is being simulated (less data) or if an actual ecosystem or geographic location is being simulated (more data). Following testing, these models have traditionally been used to improve understanding about the ecosystem components using uncertainty or sensitivity analyses of effects of changes in model parameters and drivers on model output. These results provide information that improves understanding about ecosystem behavior under alternative environmental conditions in the future and in the past. Model output can also be used to refine the theory as well as modify the model and provide feedback to data collection efforts (Ives and others 1998).

Similarities Between Traditional Approaches

The two traditional empirical and modeling approaches intersect in two ways. First, both approaches access knowledge, data, and methods (analytical, numerical models) that are readily available to the ecological community, although the degree to which data and models are used and their location-specific importance differ greatly between approaches. Second, both approaches contribute to improved understanding and ecological knowledge through publication of results, although the advances may be too site-specific in the empirical approach to be applicable to other locations, and may be too general in the theoretical approach to not actually represent any particular location (Peters and others 2012).

An Ecosystem Ecologist's Toolkit in the Era of Big Science

We propose that an integrated, iterative approach is a critical component of an ecosystem ecologists' toolkit in the modern era. This approach includes (Figure 2): (a) empirical observations to parameterize and check the reality of models or theory, (b) theoretical constructs that provide generality and constrain the parameter space for empirical observations and experiments, (c) numerical models that are integrated with analytical methods and big data analytics to efficiently use the increasing amounts

and types of data and information becoming available, and (d) increased focus on new data and information sources (for example, crowdsourcing, social media, local knowledge) that can be combined or integrated with individually collected data, federated data, and protected data that may need special handling prior to use. Many of these components already exist in many researchers' toolkits, in particular for scientists working at very fine or very broad spatial extents. But the articulation of all of the components as an integrated and iterative, actively learning approach is a novel one that we believe will allow ecosystem ecologists to take advantage of the new advances in technology needed to address global change problems.

The advantages of this new approach span and integrate all of ecosystems ecology. For instance, the new approach allows improved understanding of general principles and enables problem-solving for specific locations. The new approach can produce forecasts and backcasts for a location with documented uncertainties based on data combined with general knowledge about ecological principles. Under the new approach, conceptual and mental models can be refined through time based on an integration of empirical observations and general principles. Using the new approach, theoretical and numerical models can be challenged by the data for specific locations, and modified based on those analyses. The approach also enables empirical questions and experimental designs to be guided and informed by theoretical principles. The new approach acknowledges the importance of emerging techniques, such as those in machine learning, which can be used to maintain the integrity of the data, metadata, and findings through time so the scientific community becomes more efficient as the amount of data and new technology increase (Peters and others 2014a).

Training Ecosystem Ecologists in an Era of Big Science

Training new ecosystem ecologists in the era of Big Science presents significant challenges. Adoption of the new approach means that one may no longer be a specialist in either theoretical modeling or empirical science. Rather, it requires a generalist mindset as well as education. This is not to say that all ecosystem ecologists must be adept at all components of the discipline, but basic knowledge in how the components work (from field measurements to modeling) is required. Ideally, the ecosystem ecologists-in-training will get education and experience in many facets of the field to see how the various components can be integrated to pose and answer fundamental as well as novel ecological questions.

Going forward under the new approach, it will be necessary for ecosystem ecologists to appreciate and be familiar with the broad range of techniques used in the field. This familiarity will be necessary for one's own work and to enable effective collaboration and communication with other researchers. In addition to the traditional tools that students typically learn, such as experimental design, statistical analysis, and writing and publication of results, there are additional skills and experiences that will be required for all scientists entering the field. Some of these skills are relatively new, such as working with large geographical datasets, and some are skills that have traditionally belonged to one area (modeling or field science) that need to be taught to everyone. For instance, all students should engage in data collection to understand the complexities of the real world and the limitations of field measurements. They should also learn or become familiar with a computer programming language so that they have the tools, both practically and cognitively, to develop models or to conduct advanced big data analysis. Emerging ecosystem ecologists should also become familiar with geographical datasets that are increasingly available online across a range of spatial extents and scales of resolution. Experience in the practical tools needed to manipulate, analyze, and interpret these spatial data layers will provide insight into the uses, uncertainty, and limitations inherent in this information that is critical for understanding spatial variability in the drivers and response variables of ecosystems.

As increasing amounts of data become openly available on the internet, it is also increasingly important that ecosystem ecologists develop a critical skill in the application of skepticism towards these open access data. All data come with uncertainties and too often these limitations and assumptions are ignored when data are imported from online repositories. This skepticism is equally important when using datasets or derived data products generated by others. These uncertainties cannot be ignored or else the availability of data will become an additional way to produce inaccurate results.

Emerging ecosystems ecologists who are trained in the use of large datasets produced by models must be taught to be skeptical of these sources of information. Some of the most intriguing datasets to become openly available on the internet recently are raster datasets that offer continuous global or regional spatial coverage of one or more variables.

Similarly, there are reanalysis datasets that offer the promise of temporal records of climatic conditions in areas and eras where they were not measured. These datasets offer interpolated model-based estimates, where the errors and uncertainties may not be well-known or quantifiable. Other raster datasets provide statistical interpolations between spatial measurements, which may or may not be accurate.

Models are surrogates for a conceptual construct; thus, even apparently simple direct measurements are a form of models with uncertainties. For instance, in estimating soil moisture with a time-domain reflectometry (TDR) probe, the measurement made by the device is a voltage pulse through time. This pulse is converted, through a calibrated theoretically backed model, into soil moisture content of the soil. Any measurement which requires calibration uses a model, and failure to calibrate correctly can lead to inaccurate estimates. An example of information that is usually treated as direct measurements, but which actually comprises multiple model-derived products, are satellite estimates of surface reflectance. The actual on-board measurement can be generated on a capacitor in a charge-coupled device (CCD), which is converted through a modeled calibration to radiance, which is then converted to surface reflectance using a radiative transfer model and the model-derived estimates of atmospheric properties. The derived reflectance, as delivered, may be useful for some applications (for example, estimation of Normalized Difference Vegetation Index (NDVI); a measure of vegetation greenness), but it may be need to be treated with more caution for others (for example, derivation of surface fractions of vegetation and bare soil; Okin and Gu 2015).

A useful maxim in modeling is that ''all models are wrong, but some are useful'' (Box and Draper 1987). The first component of this saying reminds us that all models are simplifications, and cannot fully represent the world being modeled. The second component forces us to ask ''useful for what?'' A dataset generated for one purpose (for example, a global temperature reanalysis used to drive a model of plant growth) may not be compatible with another use because the model assumptions, scale, or structure differ from those in the alternate application (for example, estimating the conditions in a small experimental plot). It may be instructive to use a dataset for an incompatible use, but this must be done transparently and with skepticism.

The skepticism we teach our students is, fundamentally, based on knowledge of how the systems that we study function. However, as databases increase in spatial and temporal extent, it is increasingly difficult, if not impossible, for individuals to be familiar with the functioning of the diversity of ecosystems included in the analysis. Thus, collaboration and communication with local subject-matter experts who are familiar with both the data and their assumptions as well as how the ecosystems function will be critical for interpretation and understanding of patterns from these model-based, large, raster datasets (Peters and others 2007). In order for our quantitative and data-adept students to be able to effectively communicate with these local experts, their analyses must remain grounded in empirical reality and square with knowledge and intuition derived through deep understanding of process and pattern in real ecosystems. Thus, we repeat our call for students doing big data analysis to also have familiarity with the real world through making actual measurements.

Conclusions

As the amount of data, derived data products, and information increase with advances in technology, and our world becomes increasingly connected via communication to both scientific and non-technical audiences globally, it will be increasingly important that ecosystem ecologists have a toolkit that can handle this technology and connectivity. We described one approach that takes advantage of the strengths of empirical, theoretical, and numerical modeling approaches to understanding and predicting ecosystem dynamics. The integrated, iterative approach with learning provides advantages over traditional approaches through improved: (a) understanding of general principles and problem-solving for specific locations; (b) forecasts and back-casts for locations with documented uncertainties; (c) conceptual and mental models; (d) theoretical and numerical models; (e) empirical questions and experimental design; and (f) scientific efficiency through machine learning. This new approach requires additional training for students and an education that includes tools from across the discipline. While new skills will enable effective research with emerging large datasets, the need for familiarity with real ecosystems and real measurements combined with collaboration with local experts are required to ground the use and treatment of these sources of information. In addition, a healthy dose of skepticism is needed to temper and inform the use of online, open access datasets emerging from a more connected, measured, and modeled world.

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