ABSTRACT

One of the pillars of the modern scientific method is model validation: comparing a scientific model’s predictions against empirical observations. Today, a scientist demonstrates the validity of a model by making an argument in a paper and submitting it for peer review, a process comparable to code review in software engineering. While human review helps to ensure that contributions meet high-level goals, software engineers typically supplement it with unit testing to get a more complete picture of the status of a project.

We argue that a similar test-driven methodology would be valuable to scientific communities as they seek to validate increasingly complex models against growing repositories of empirical data. Scientific communities differ from software communities in several key ways, however. In this paper, we introduce SciUnit, a framework for test-driven scientific model validation, and outline how, supported by new and existing collaborative infrastructure, it could integrate into the modern scientific process.

Categories and Subject Descriptors
D.2.5 [Software Engineering]: Testing and Debugging
Documentation, Measurement, Standardization

Keywords
unit testing, model validation, cyberinfrastructure

1 INTRODUCTION

Scientific theories are increasingly being organized around quantitative models: formal systems capable of generating predictions about observable quantities. A model can be characterized by its scope: the set of observable quantities that it attempts to predict, and by its validity: the extent to which its predictions agree with experimental observations of these quantities.

Today, quantitative models are validated by peer review. For a model to be accepted by a scientific community, its advocates must submit a paper that describes how it works and provides evidence that it makes more accurate predictions than previous models (or that it makes a desirable tradeoff between accuracy and complexity) [2]. Other members of the relevant community are then tasked with ensuring that validity was measured correctly and that all relevant data and competing models were adequately considered, drawing on knowledge of statistical methods and the prior literature. Publishing is a primary motivator for most scientists [3].

Quantitative scientific modeling shares much in common with software development. Indeed, quantitative models are increasingly being implemented in software and in some cases, the software is the model (e.g., complex simulations). The peer review process for papers is similar in many ways to the code review process used in many development teams, where team members look for mistakes, enforce style and architectural guidelines and check that the code is valid (i.e., that it achieves its intended goal) before permitting it to be committed to the primary source code repository.

Code review can be quite effective [10], but this requires that developers expend considerable effort [6]. Most large development teams thus supplement code reviews with more automated approaches to verification and validation, the most widely-used of which is unit testing [1]. In brief, unit tests are functions that check that the behavior of a single component satisfies a single functional criterion. A suite of such tests complements code review by making it easier to answer questions like these:

1. What functionality is a component expected to have?
2. What functionality has been adequately implemented? What remains to be done?
3. Does a candidate code contribution cause regressions in other parts of a program?

Scientists ask analogous questions:

1. What is a model’s scope and how is validity measured?
2. Which observations are already explained by existing models? What are the best models of a particular quantity? What data has yet to be explained?
3. What affect do new observations have on the validity of previously published models? Can new models explain previously published data?

But while software engineers can rely on a program’s test suite, scientists today must extract this information from a body of scientific papers. This is increasingly difficult. Each paper is narrowly focused, often considering just one model or dataset, and is frozen in time, so it does not consider the latest models, data or statistical methods. Discovering, precisely characterizing and comparing models to determine the state of the art and find open modeling problems can require an encyclopedic knowledge of the literature, as can

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logic developed alongside traditional peer review. However, process could be improved by adoption of test-driven

caricature, this motivates our suggestion that the scientific

can be overwhelming [4], and comprehensive reviews of

finding all data relevant to a model. Senior scientists often

attempts to fill these needs by publishing review papers, but

in many areas, the number of publications generated every

year can be overwhelming [4], and comprehensive reviews of

a particular area are published infrequently. Statisticians of-
ten complain that scientists are not following best practices

and that community standards evolve too slowly because a
canonical paper or popular review relied on outdated meth-

ods. Furthermore, if the literature simply doesn’t address

an important question of validity (e.g. if space was limited),
a researcher might need to reimplement an existing model

from scratch to attempt to address it.

One might compare this to a large software development
team answering the questions listed above based largely on
carefully reviewed, but rarely updated, API documentation
and annual high-level project summaries. While certainly a
caricature, this motivates our suggestion that the scientific
process could be improved by the adoption of test-driven
methodologies alongside traditional peer review. However, the
scientific community presents several unique challenges:

1. Unit tests are typically pass/fail, while goodness-of-fit
between a model and data is typically measured by a
continuous metric.

2. Unit tests often test a particular component, whereas
a validation testing system must be able to handle and
compare models with the same scope.

3. Scientists use a variety of programming languages.

4. Scientists often only loosely coordinate their efforts.

5. Different communities, groups and individuals prefer
different goodness-of-fit metrics and focus on different
sets of observable quantities. In contrast, there is more
pressure to agree upon requirements and priorities in
a typical software development project.

6. Professional software developers are typically trained
in testing practices and the use of collaborative tools,
while scientists more rarely have such experience [9].

To begin to address these challenges, we will introduce a lightweight and flexible validation testing and framework
called SciUnit in Sec. 2. Many of these challenges have to
do with coordination between scientists. To begin to ad-
dress this, we then describe a community workflow based
on widely-adopted social coding tools (here, Github) and a
lightweight community portal called SciDash, in Sec. 3. The
overall goal of this work is to help scientists generate tables
like the one central to Figure 1, where the relative validity of
a set of models having a common scope can be determined
by examining scores produced by a suite of validation tests
constructed from experimental data. We discuss adoption
strategies and conclude in Sec. 4 with directions for future
research into scientific model validation practices.

2 VALIDATION TESTING WITH SCIUNIT

As a motivating example, we will begin by considering a
community of early cosmologists recording and attempting
to model observations of the planets visible in the sky, such
as their position, velocity, orbital eccentricity and so on. One
canonical test might ask a model to predict planetary
position on night \(n+1\) given observations of its position on
\(n\) previous nights. Figure 2 shows how to implement a test,
using SciUnit, that captures this logic.

Before explaining the details of this example, we point out
that SciUnit is implemented in Python. Python is one of the
most widely used languages in science today [8], and is in-
creasingly regarded as the de facto language of open source
scientific computing. It is easy to read and has a simple
object system that we use to specify the interface between
tests and models (challenge 2, see below). It supports calling
into other popular languages, including R, MATLAB, C
and Java, often more cleanly than they support calling into
Python (challenge 3). The IPython notebook is a powerful
web-based “read-eval-visualize loop” that we will use to
support interactive table visualization, and it also permits
using other languages on a per-cell basis [7]. Together, this
class PositionTest(sciunit.Test):
    """Tests a planetary position model based on positions observed on night n given the positions in the n-1 previous nights.
    """
    Observation = f
    'histories': list[list[Position]],
    'positions': list[Position]
    return pool_position

def generate_prediction(self, model):
    return model.predict_next_pos(obs_history)

def compute_score(self, observation, prediction):
    obs_positions = observation['positions']
    return pooled_p_val([abs_distance(obs, pred) for (obs, pred) in zip(obs_positions, prediction)])

Figure 2: An example test class in cosmounit.

makes writing wrappers around tests and models written in other languages relatively simple. We anticipate making it nearly automatic as future work.

A SciUnit validation test is an instance of a Python class inheriting from sciunit.Test (line 1). Every test takes one required constructor argument (inherited from the base class): the observation(s) against which the test will validate models. In our example, this is a dictionary, documented per Python conventions on lines 2-6. To create a particular position test, we instantiate this class with particular observations. For example, the subset of cosmologists interested specifically in Saturn might instantiate a test by randomly chunking observations made about Saturn’s nightly position over time as follows:

```python
h, p = randomly_chunk(obsd_saturn_positions)
saturn_position_test = PositionTest(
    {'histories': h, 'positions': p})
```

The class PositionTest defines logic that is not specific to any particular planet, so it is contained in a repository shared by all cosmologists called cosmounit. The particular test above would be constructed in a separate repository focused specifically on Saturn called saturnsuite. Both would be collaboratively developed by these (overlapping) research communities in source code repositories on Github.

Classes that implement the sciunit.Test interface must specify two methods: a method for extracting a prediction from a model, and a method for producing a score from that prediction. Predictions are extracted by a separate method to make it easier for statisticians to write new tests for which only the goodness-of-fit metric differs, not the method by which the prediction is extracted (challenge 5).

The generate_prediction method (lines 8-11) is passed a model as input and must extract a prediction. A model is an instance of a class inheriting from sciunit.Model and a prediction can be any Python data structure. To specify the interface between the test and the model, the test class specifies a list of required_capabilities (line 7). A capability specifies the methods that a test may need to invoke on the model to extract a prediction, and is analogous to an interface in a language like Java. In Python, capabilities are written as classes with unimplemented members, shown in Figure 3. Classes defining capabilities are tagged as such by inheriting from sciunit.Capability. The test in Figure 2 repeatedly uses this capability on lines 9-11 to return a list of predicted positions for each observed history (using a list comprehension for brevity). A planet’s position is represented using a standard celestial coordinate system specified within cosmounit by the class Position.

A model class implements a capability by inheriting from it and implementing the required methods (Figure 3). The scope of a model class is identified by the capabilities it has. A particular model is an instance of such a class:

```
lin_saturn_model = LinearPlanetModel()
```

Once a prediction has been extracted from a model, the test class must compute a score. The framework invokes the compute_score method with the observation provided upon test instantiation and the prediction just generated. On lines 13-17 of Fig. 2, the test class constructs a list of distances between the observed and predicted positions, then determines a pooled p-value to determine the goodness-of-fit (the details are omitted for concision). A p-value is represented as an instance of sciunit.PValue, a subclass of sciunit.Score that has been included with SciUnit due to its wide use across science.

This illustrates a key difference between unit testing, which would simply produce a boolean result, and our conception of scientific validation testing (challenge 1). A score class must induce an ordering, so that a table like that shown in Figure 1 can be sorted along its columns. A score class can also specify a normalization scheme so the cells of the table can be color-coded.

The judge method of a test can be invoked to compute a score for a single model:

```
score = saturn_position_test.judge(lin_saturn_model)
```

This method first checks that the model implements all required capabilities, then calls the generate_prediction method, then passes the prediction to the compute_score method. A reference to the test, model, observation, prediction and other related data the test provides (none here) are added as attributes of the score before it is returned.

To produce a comprehensive test suite, the contributors to saturnsuite would instantiate a number of other tests and then create an instance of the TestSuite class:

```
saturn_motion_suite = sciunit.TestSuite(
    saturn_position_test, saturn_velocity_test, ...
)
```

They would also instantiate a number of models. A test suite can be used to judge multiple models at once, if they satisfy the union of the capabilities required by the constituent tests (challenge 2). The result is a score matrix:

```
sm_matrix = saturn_motion_suite.judge(
    lin_saturn_model, ptolemy_model, kepler_model, ...
)
```

If constructed inside an IPython notebook, a score matrix can then be visualized as an interactive table, much like the one shown in Figure 1. Scientists can sort by column and click on tests, models and scores to get more information on each, including documentation, authorship information, related papers and other related data extracted from the underlying classes (details omitted for concision).
3 COLLABORATIVE WORKFLOW

Social coding tools like GitHub allow each scientist to work on their own fork of a repository like `saturnunit` where they can examine the consequences of their own contributions on the tests and models that have previously been developed. For example, an experimentalist who has gathered new data can instantiate a new test or refine an existing one with more accurate observations. As long as the interface between the test and the model remains the same, the scores for prior models can be recomputed entirely automatically, requiring no coordination with model developers (challenge 4). When a modeler develops a new model, she can validate it against all the tests it is capable of taking. If a statistician develops a better goodness-of-fit metric, she too can use existing capabilities and indeed inherit prediction extraction logic directly, as discussed above. If a scientist is not interested in certain tests, she can locally remove them to recalibrate her view of the relative merits of different models (challenge 5).

If the changes to the repository appear to represent a contribution, these scientists might submit a pull request to the central repository (either separately or together with the submission of a conventional paper). Anonymous reviewers tasked by the “editors” of the repository would then subject the pull request to appropriate peer review before committing it to the “permanent record”. A model that performs well across tests in a collaboratively developed suite could more objectively claim (e.g. to reviewers) to be a coherent, valid model of, for example, Saturn’s motion.

To help scientists discover and coordinate development of these repositories, we are developing a collaborative portal called SciDash (http://scidash.org/). It is essentially a wiki pointing scientists to the repositories designated as “primary” by early adopters in their research areas (who may serve as de facto initial editors as well). SciDash also supports loading IPython notebooks containing score tables stored in these repositories into the browser, avoiding the need to clone the repository locally. To modify the suite (e.g. to add the model a scientist is developing to it), a scientist can simply fork the repository by clicking a button at the top of this view. We are exploring ways of loading forks directly into a cloud-based IPython notebook system, so that the complexities of Git, Python setup and package management can be left behind the scenes (challenge 6). SciDash lists public forks of repositories that it is indexing to help scientists get a better sense of who is working on the problems they are interested in and what partial results are publicly available, fostering collaboration.

As with many pieces of cyberinfrastructure, early adopters may benefit less than late adopters due to network effects. To incentivize adoption, we look to an increasingly common solution that makes sense: modeling competitions. Many research communities use these to periodically determine the state of the art, resulting in a form of review paper (e.g. [5]). Funding sources often include small monetary incentives. SciDash could be used to run these kinds of competitions on a continuous basis atop less ad hoc infrastructure (and thus require less effort and central planning from organizers) and we are actively recruiting organizers for such competitions.

4 DISCUSSION & FUTURE DIRECTIONS

Instead of attempting to use an existing general-purpose testing framework (e.g. JUnit or PyUnit), we have designed what is essentially a domain-specific language that captures the scientific model validation process in more familiar terms (in view of challenge 6).

While we discuss a simple example based on planetary movement here, we have applied this framework to more realistic problems in neurobiology in collaboration with the developers of two large-scale informatics projects, OpenSourceBrain and NeuroElectro, which serve as a source of models and data, respectively. Our tools serve, in essence, as a bridge between these resources. The tools we describe could also be used for a variety of other scientific disciplines, including within software engineering to validate predictive models of, for example, project duration or code reuse.

This work identifies new research directions in software engineering by developing connections between test-driven development [1] and the scientific model validation process, which has not been as extensively studied. Characterizing how scientists today attempt to answer the questions given in the introduction, evaluating how well sociotechnical solutions like the ones we propose here could improve their ability to do so, and studying adoption barriers are likely to be fruitful avenues for future empirical research, and lead to a better understanding of both programmers and scientists.

The core SciUnit framework has been fully developed and is available at http://scunit.scidash.org/. SciDash is under active development as of this writing.

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6 REFERENCES