Collaborative Infrastructure for Test-Driven Scientific Model Validation

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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, particularly when it is complex and involves many contributors.

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 SciUnit, supported by new and existing collaborative infrastructure, could be integrated into the modern scientific workflow.

Categories and Subject Descriptors

D.2.5 [**Software Engineering**]: Testing and Debugging

General Terms

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.

Quantitative models are today validated by *peer review*. For a model to be accepted by a scientific community, its advocates must submit a paper describing how it works and providing evidence that it predicts a quantity of interest more accurately than previous models, or in some cases, that it makes a desirable tradeoff between accuracy and complexity [1]. Other members of the relevant community are then tasked with ensuring that validity was measured properly and that relevant data and competing models were adequately considered, drawing on knowledge of statistical methods and on the prior literature. Publishing is a primary motivator for most scientists [2].

Quantitative scientific modeling and software development share much in common. 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.

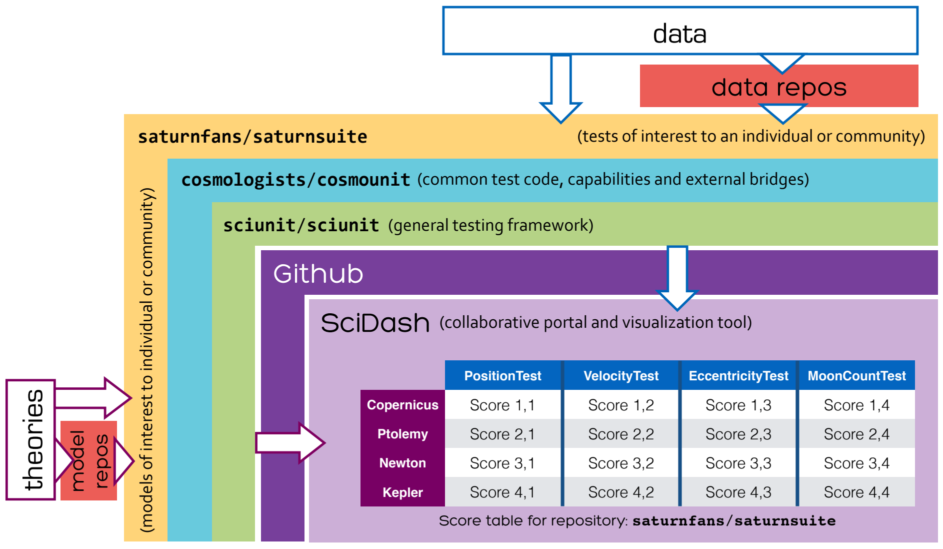
Code review can be quite effective [3], but this requires that developers expend considerable effort [4]. Most large development teams thus supplement code reviews with more automated approaches to verification and validation, the most widely-used of which is *unit testing* [5]. In brief, unit tests 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 more easily:

1. What functionality should each component 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 analagous questions:

1. What are the contemporary community standards for measuring goodness-of-fit?
2. Which observations are already explained by existing models? What are the best models? What are the open modeling problems of interest?
3. How do newly-made experimental observations impact 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 publications. This is increasingly difficult. Each publication focuses on just one model and is frozen in time, so it does not consider the latest experimental data or statistical methods. Discovering, precisely characterizing


data
data repos
saturnfans/saturnsuite
(tests of interest to an individual or community)
cosmologists/cosmounit (common test code, capabilities and external bridges)
sciunit/sciunit (general testing framework)
Github
SciDash (collaborative portal and visualization tool)
theories
model repos
(models of interest to individual or community)
Score table for repository: saturnfans/saturnsuite

	PositionTest	VelocityTest	EccentricityTest	MoonCountTest
Copernicus	Score 1,1	Score 1,2	Score 1,3	Score 1,4
Ptolemy	Score 2,1	Score 2,2	Score 2,3	Score 2,4
Newton	Score 3,1	Score 3,2	Score 3,3	Score 3,4
Kepler	Score 4,1	Score 4,2	Score 4,3	Score 4,4

Figure 1: Tests are derived from data and models are derived from scientific theories. The score table summarizes the performance of a collection of models against a suite of tests. A table is generated and visualized in an IPython notebook stored inside a *suite repository* (e.g. `saturnsuite`) hosted on social coding infrastructure (here, Github). SciDash is a portal that discovers and organizes these suite repositories and provides read-only views of the notebooks they contain. Common testing code, capabilities and bridges to external model and data repositories are also collaboratively developed in *common repositories* (e.g. `cosmounit`).

and comparing models to discover the state of the art and find open modeling problems can require an encyclopedic knowledge of the literature, as can finding all data relevant to a model. Senior scientists often attempt to fill this need by publishing review papers, but in many areas, the number of publications generated every year can be overwhelming [6], and comprehensive reviews of a particular area are published relatively infrequently. Statisticians often complain that scientists are not following best practices and that community standards evolve too slowly because a canonical paper or popular review used outdated methods. Furthermore, if the literature simply doesn't address an important question of validity, because new data has been gathered since the model paper was published for example, a researcher might need to reimplement an existing model in order to evaluate it.

One might compare this to a large software development team answering the questions listed above based only on carefully reviewed component documentation together with annual high-level project summaries. Although 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 that must be addressed by any such methodology:

1. Unit tests are typically pass/fail, while goodness-of-fit between a model and data is typically measured by a continuous metric (e.g. a p-value).
2. Unit tests often test a *particular* component, whereas a *validation test* must be able to handle and compare many models capable of predicting the same quantity.
3. Different modelers use different programming languages.
4. Professional software developers are typically trained in testing practices and tools, while scientists rarely have training or experience with testing practices [7]. Thus, the framework must be as simple as possible.
5. Different communities, groups and individuals prefer different goodness-of-fit metrics and care about different sets of observable quantities. In contrast, there is typically more pressure to agree upon requirements and priorities in a software development project.

To address challenges 1-4, we will introduce a lightweight scientific validation testing framework, *SciUnit*, in Sec. 2. Challenge 5 has to do with coordination between scientists. To address this, we introduce a community workflow based on widely-adopted social coding tools (here Github) along with a lightweight community portal called *SciDash*. The overall goal of this work is to help scientists generate and examine 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.

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 simple validation 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]. It supports calling into many of the other popular languages, including R, MATLAB, C and Java, more cleanly than these languages support calling into Python (challenge 3). It is widely-recognized as being easy-to-read and its object system can be used to define abstract interfaces, which we leverage in support of challenge 2.

A *SciUnit* validation test is an instance of a Python class

```
1  class PositionTest(sciunit.Test):
2      """Tests a planetary position model based on
           positions observed on day n given the
           positions in the n-1 previous days.
3      Metric: Standard p-value.
4      Parameters:
5        obs_histories : list[list[position]]
6        obs_positions: list[position]"""
7    def __init__(self, obs_histories, obs_positions):
8      self.obs_histories = obs_histories
9      self.obs_positions = obs_positions
10
11   required_capabilities = [PredictsPlanetaryPosition]
12
13   def _judge(self, model):
14     predictions = []
15     for obs_history in self.obs_histories:
16       predictions.append(model.predict_next_pos(
             obs_history))
17     p = pooled_p_val(predictions, self.obs_positions)
18     return sciunit.PValue(p, related_data={
19       'obs_histories': obs_histories,
20       'obs_positions': obs_positions,
21       'predictions': predictions
22     })
```

Figure 2: An example test class in `cosmounit`.

implementing the `sciunit.Test` abstract interface (line 1). Here, the class `PositionTest` takes two *parameters* in its constructor (constructors are named `__init__` in Python, lines 7-9). The meaning of each parameter along with a description of the goodness-of-fit metric used by the test is documented on lines 2-6. To create a *particular* position test, we instantiate this class with particular planetary observations. For example, the subset of cosmologists interested specifically in Saturn might instantiate a test by randomly chunking observations made about Saturn as follows:

```
h, p = randomly_chunk(saturn_obs_positions)
saturn_position_test = PositionTest(h, p)
```

The class `PositionTest` defines logic that is not specific to any particular planet, so it is contained in a package shared by all cosmologists called `cosmounit`, while the particular test above would be used in a test suite focused specifically on Saturn called `saturnsuite`. Both the common logic and specific suites are collaboratively developed by these overlapping research communities in source code repositories on Github (or another similar service).

Classes that implement the `sciunit.Test` interface must contain a `_judge` method that receives a candidate *model* as input and produces a *score* as output. To specify the interface between the test and the model, the test author provides a list of *capabilities* in the `required_capabilities` attribute, seen on line 11 of Fig. 2. Capabilities are simply collections of methods that a test will need to invoke in order to receive relevant data, and are analogous to *interfaces* in e.g. Java. In Python, capabilities must be written as classes with unimplemented members. The capability required by the test in Figure 2 is shown in Figure 3. In *SciUnit*, classes defining capabilities are tagged as such by inheriting from `sciunit.Capability`. The test in Figure 2 repeatedly uses this capability on line 16 to produce a position prediction for each observation. We assume that positions are represented in a standardized manner specified within `cosmounit`. A model is simply an object that implements capabilities (via Python's simple inheritance mechanism).

The remainder of the `_judge` method compares the model predictions to observed data to produce a pooled p value. The method returns an instance of `sciunit.PValue`, a sub-

```
class PredictsPlanetaryPosition(sciunit.Capability):
  def predict_next_pos(self, history):
    """Takes a list of previous positions and produces
       the next position."""
    raise NotImplementedError("Model does not
        implement capability.")
```

Figure 3: An example capability specifying a single required method (used by the test in Figure 2).

class of `sciunit.Score` that has been included with *SciUnit* due to its generality. In addition to the p-value itself, the returned score object also contains metadata, via the `related_data` parameter, for scientists who may wish to examine the result in more detail later. This illustrates some key differences between unit testing, which would simply produce a boolean result, and our conception of scientific validation testing (challenge 1). A score must induce an ordering, so that the table shown in Figure 1 can be sorted along its columns, and it can optionally specify a normalization scheme so the cells can be color-coded (not shown). A test can be manually executed using the `judge` method:

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

This method proceeds by first checking that the provided model implements all required capabilities before calling the test's `_judge` method to produce a score. A reference to the test and model are added to the score for convenience (accessible via the `test` and `model` attributes, respectively).

Alongside this position test, we could also provide a number of other test classes in `cosmounit` and instantiate them with data about aspects of Saturn's motion (e.g. it's velocity) to produce a comprehensive suite in `saturnsuite`.

```
saturn_motion = sciunit.TestSuite([
    saturn_position_test, saturn_velocity_test, ...])
```

Like a single test, a test suite is capable of judging one or more models. The result is a score matrix much like the one diagramed in Fig. 1.

```
sm_matrix = saturn_motion.judge([copernicus_sat,
    ptolemy_sat, newton_sat, kepler_sat])
```

A test suite requires the union of the capabilities required by the tests it contains. A model that performs well across tests in such a suite could reasonably claim (e.g. to reviewers) that it is a coherent, valid model of Saturn's motion. As new data is collected, new tests can be added to the suite. However, because the interface between the test and the model remains the same (only the data parameterizing the tests changes), the table can be updated automatically. Similarly, when a new model is developed, it can immediately be evaluated against all known data that has been encoded as a test by simply exposing its predictions via the capabilities the test requires.

3 Collaborative Workflow

The design just described has been purposefully left as simple as possible, in pursuit of challenge 4. Despite its simple design, it captures the essential elements of the scientific model validation process and satisfies the four challenges we laid out. SciUnit can be used by individual scientists to organize their workflows, but because science, and in particular, model validation is a collaborative process, we have also described the intended use of SciUnit within a collaborative workflow, mediated by a social coding tool like Github.

More directly: we anticipate common testing logic (e.g. `PositionTest`), modeling logic and capabilities being collaboratively developed by larger communities in less specialized repositories like `cosmounit`. Individuals and small groups will then parameterize these tests and models with data they have gathered, as well as data known from the literature and data contained in existing data repositories to create test suites in repositories like `saturnsuite`. The interface between data collection software and existing data representation standards and tests will be mediated by bridge logic also contained in repositories like `cosmounit`.

Statisticians wishing to promote new validation metrics can simply for a X`unit` repository and implement new test logic. By reusing the same interfaces as previous tests used, these new metrics can immediately be used to validate or invalidate a large body of existing models, providing valuable data for use in convincing the community to adopt these into the mainstream repositories. Similarly, investigators who wish to de-emphasize or emphasize different quantities can fork X`suite` repository and add or remove tests.

To help organize these repositories, a simple collaborative portal sitting above Github called *SciDash* is currently under development (*http://scidash.org/*). SciDash consists of an organized, collaboratively filtered listing of X`unit` and X`suite` repositories. That is, it is a tool to help scientists find the most popular repositories in their research area, to facilitate the development of community standards. SciDash also supports extracting summaries of tests, models, scores and related data from suite repositories to generate hyperlinked score tables and documentation. This facilitates exploratory workflows. To modify a suite (e.g. by adding the model a scientist is developing to it), a scientist can simply fork the repository. SciDash automatically discovers public forks of repositories that it is already indexing.

4 Discussion

Academic peer review and code review are similar, but software developers typically supplement human review with test-driven methodologies. Such methodologies may benefit scientific communities as well, but several unique constraints make reusing existing testing frameworks and processes difficult. We describe a core testing framework that addresses these issues by using an existing, widely-adopted language and designing a flexible, simple framework that captures the domain-specific structure of scientific model validation. We then describe, by example, how the various components can be organized into software repositories and collaboratively maintained using social coding tools to support existing scientific practices. We end by outlining a collaboratively filtered portal that sits atop these tools and facilitates exploratory analyses and repository discovery.

While we discuss a toy example based on planetary movement here, we have applied this framework to more realistic problems in neurobiology and have bridged SciUnit to large-scale neuroinformatics projects (we anticipate publishing a description of these case studies shortly). Much future work remains to be done to investigate whether these tools are truly usable and useful to scientific communities, to further develop the community workflow and infrastructure and to develop a range of realistic case studies. Nevertheless, we believe that identifying the synergies between testing practices and model validation, and describing the basic tooling, represents a novel contribution to the literature on software testing. The core SciUnit framework has been fully developed and is available at http://sciunit.scidash.org/. SciDash is under active development, and is currently capable of basic forms of the operations described in Sec. 3.

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