Test Driven Development of Scientific Models

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Outline

1 Motivations
2 Testing
3 Testing Frameworks
4 Test-driven Development (TDD)
5 What about numerical software?
Motivation 1: Fear/Stress
Motivation 1: Fear/Stress

photomatt7.wordpress.com
Motivation 1: Fear/Stress
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Calvin & Hobbes - Bill Waterson
Motivation 2: Productivity

Change

Verify
Motivation 2: Productivity

- New feature
- Refactor

Change  Verify
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Compiles?
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Compiles?
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Change -> Verify

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Verify

- Compiles?
- Executes?
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What is the latency of verification for large scientific models?
Some observations about human behavior:

- Risk of defects scales with magnitude of change per iteration
- Development time per iteration will be comparable to verification time
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Conclusion:

**Productivity is a nonlinear function of the cost of verification!**
Motivation 3: The Limelight

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- Strong validation against data, but ...

\(^1\)Pearce, Fred. “Top economist counts future cost of climate change.”
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  - Those which change results below detection threshold

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Test Harness - work in safety

Collection of tests that constrain system
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- Localizes defects
- Improves developer confidence
- Decreases risk from change
- Inexpensive compared to application (ideally)
Do you write legacy code?
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Michael Feathers

*Working Effectively with Legacy Code*
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“Fear is the path to the dark side. Fear leads to anger. Anger leads to hate. Hate leads to suffering.” - Yoda

starwars.wikia.com
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*Working Effectively with Legacy Code*

- Lack of tests leads to fear of introducing subtle bugs and/or changing things inadvertently.
- Also is a barrier to involving pure software engineers in the development of our models.
Excuses, excuses ...
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  http://java.dzone.com/articles/unit-test-excuses
  - James Sugrue

- Numeric/scientific code cannot be tested, because …
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- Clear intent
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4. Test-driven Development (TDD)
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Testing Frameworks

- Framework Driver
- User Tests
- Framework Services
- Application

Report:
1271 tests run
2 Failures
Testing Frameworks

- Key services
  - Provide methods to succinctly express expected values
    ```python
call `assertEqual(120, factorial(5))`
  ```
  - Register test procedures with framework
  - Execute test procedures, and summarize success/failure
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    call assertEqual(120, factorial(5))
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  - Register test procedures with framework
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- Generally specific/customized to programming language (xUnit)
  - Java (JUnit)
  - Python (pyUnit)
  - C++ (cxxUnit, cppUnit)
  - Fortran (FRUIT, FUNIT, pFUnit)
Frameworks and IDE's

Frameworks are often integrated within IDEs for even greater ease of use:
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Today I am here to sell you something ...
Old paradigm:
- Tests written by separate team (black box testing)
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Consequences:
- Testing schedule compressed for release
- Defects detected late in development ($$)
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New paradigm - Test-driven development (TDD)
- Developers write the tests (white box testing)
- Tests written before production code
- Enabled by emergence of strong unit testing frameworks
The TDD cycle

- Extend Tests
- Fix/Extend Production Code
- Run Tests
- Success?
- Refactor

Focus on interface

Focus on algorithm

Pass

Fail
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- **High quality implementation?**
  - Emphasis on interfaces
  - Testable code is cleaner code.
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Unique testing challenges of numerical software
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- Presence of numerical error (roundoff or truncation)
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- Stability - issues that occur after long integrations
- Emergent properties of coupled systems (including stability)
Numerical error

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- Error estimates are seldom available for complex algorithms
- Best case scenario is usually some asymptotic form with unknown leading coefficient!
TDD techniques in presence of numerical error
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Sources:
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1. Approximation
TDD techniques in presence of numerical error

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TDD techniques in presence of numerical error

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Mitigation strategies:
TDD techniques in presence of numerical error

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Mitigation strategies:
1. Approximation:
   ▶ Test the implementation not the math (i.e., duck)
   ▶ Often more appropriate as validation test
TDD techniques in presence of numerical error

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Mitigation strategies:

- Approximation:
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- Nonlinearity - use tailored synthetic inputs:
  - E.g., choose values to make denominators $O(1)$
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Mitigation strategies:

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   - Often more appropriate as *validation* test
2. Nonlinearity - use tailored synthetic inputs:
   - E.g., choose values to make denominators O(1)
3. Composition/iteration: test steps in isolation:
   - Allows choice of tailored synthetic inputs at each step
   - Test iteration *logic* not *accumulation*
Example - testing layers in isolation

Consider the main loop of a climate model:

**Do test**
- Proper # of iterations
- Pieces called in correct order
- Passing of data between components

**Do NOT test**
- Calculations inside components

Easier with *objects* than with procedures.
TDD without “known” solutions

Consider the apparent contradiction:
TDD without “known” solutions

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- Complex algorithms yield few nontrivial analytic solutions.
- Implementations are not random keystrokes
TDD without “known” solutions

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- Apparently analytic solutions are unnecessary!
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Tests should only verify translation, not validity of algorithms
- Test each step in isolation
- Tailor synthetic inputs to yield “obvious” results for each step
- Separately test that steps are composed correctly
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But still use high level analytic solutions as tests when available!
TDD and irreducible complexity

“Aren’t my tests as complex as the implementation?”
“Aren’t my tests just repeating logic in the implementation?”
TDD and irreducible complexity

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TDD and irreducible complexity

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  - *Models couple* many components/algorithms ⇒ *exponential complexity*
  - Tests are *decoupled* ⇒ *linear complexity*
TDD and emergent properties

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- At the very least, TDD can reduce the frequency with which one must perform long integrations
TDD and performance

- TDD emphasizes small fine-grained implementations
- Such implementations are often sub-optimal in terms of performance
- Optimized implementations typically fuse multiple operations
TDD and performance

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- Such implementations are often sub-optimal in terms of performance
- Optimized implementations typically fuse multiple operations
- Solution: bootstrapping
  - Use initial TDD solution as unit test for optimized implementation
  - Maintain both implementations (and tests)
TDD and the burden of legacy code

- TDD was created for developing new code, and does not directly speak to testing legacy code.
- Best practice for incorporating new functionality:
  - Avoid wedging new logging directly into existing large procedure
  - Use TDD to develop separate facility for new computation
  - Just call the new procedure from the large legacy procedure
- Refactoring
  - Use unit tests to constrain existing behavior
  - Very difficult for large procedures
  - Try to find small pieces to pull out into new procedures
Acknowledgements

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Summary

- TDD can be applied to scientific models
- Tool support exists (unabashed plug for pFUnit tutorial)
- Cost/benefit analysis for numerical software needs further study

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Test-Driven Development: By Example - Kent Beck