Study Guide: Scientific software engineering for a simple ODE problem

Hans Petter Langtangen[1,2]

[1]Center for Biomedical Computing, Simula Research Laboratory
[2]Department of Informatics, University of Oslo

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Contents

1 Creating user interfaces

- Never edit the program to change input!
- Set input data on the command line or in a graphical user interface
- How is explained next

1.1 Accessing command-line arguments

- All command-line arguments are available in `sys.argv`
- `sys.argv[0]` is the program
- `sys.argv[1:]` holds the command-line arguments
- Method 1: fixed sequence of parameters on the command line
- Method 2: `-option value` pairs on the command line (with default values)

```
Terminal> python myprog.py 1.5 2 0.5 0.8 0.4
Terminal> python myprog.py --I 1.5 --a 2 --dt 0.8 0.4
```

1.2 Reading a sequence of command-line arguments

The program `decay_plot_mpl.py`[1] needs this input:

- I
- a
- T
- an option to turn the plot on or off (`makeplot`)
- a list of Δt values

Give these on the command line in correct sequence

```
Terminal> python decay_cml.py 1.5 2 0.5 0.8 0.4
```

1.3 Implementation

```
import sys

def read_command_line():
    if len(sys.argv) < 6:
        print 'Usage: %s I a T on/off dt1 dt2 dt3 ...' % \
              sys.argv[0]; sys.exit(1)  # abort

    I = float(sys.argv[1])
    a = float(sys.argv[2])
    T = float(sys.argv[3])
    makeplot = sys.argv[4] in ('on', 'True')
    dt_values = [float(arg) for arg in sys.argv[5:]]

    return I, a, T, makeplot, dt_values
```

Note:

[1] http://tinyurl.com/jvzzcfn/decay/decay_plot_mpl.py

- `sys.argv[i]` is *always a string*
- Must explicitly convert to (e.g.) `float` for computations
- List comprehensions make lists: `[expression for e in somelist]`

Complete program: `decay_cml.py`[2].

1.4 Working with an argument parser

Set option-value pairs on the command line if the default value is not suitable:

```
Terminal> python decay_argparse.py --I 1.5 --a 2 --dt 0.8 0.4
```

Code:

```
def define_command_line_options():
    import argparse
    parser = argparse.ArgumentParser()
    parser.add_argument('--I', '--initial_condition', type=float,
                        default=1.0, help='initial condition, u(0)',
                        metavar='I')
    parser.add_argument('--a', type=float,
                        default=1.0, help='coefficient in ODE',
                        metavar='a')
    parser.add_argument('--T', '--stop_time', type=float,
                        default=1.0, help='end time of simulation',
                        metavar='T')
    parser.add_argument('--makeplot', action='store_true',
                        help='display plot or not')
    parser.add_argument('--dt', '--time_step_values', type=float,
                        default=[1.0], help='time step values',
                        metavar='dt', nargs='+', dest='dt_values')
    return parser
```

(`metavar` is the symbol used in help output)

1.5 Reading option-values pairs

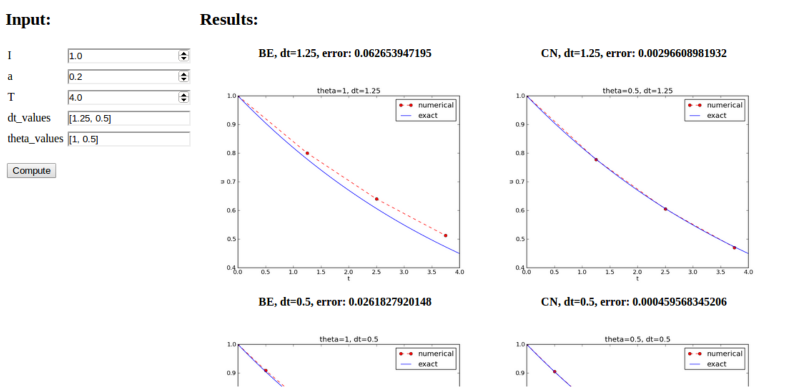
`argparse.ArgumentParser` parses the command-line arguments:

```
def read_command_line():
    parser = define_command_line_options()
    args = parser.parse_args()
    print 'I={}, a={}, T={}, makeplot={}, dt_values={}'.format(
        args.I, args.a, args.T, args.makeplot, args.dt_values)
    return args.I, args.a, args.T, args.makeplot, args.dt_values
```

Complete program: `decay_argparse.py`[3].

[2] http://tinyurl.com/jvzzcfn/decay/decay_cml.py
[3] http://tinyurl.com/jvzzcfn/decay/decay_argparse.py

1.6 A graphical user interface



Normally very much programming required - and much competence on graphical user interfaces. Here: use a tool to automatically create it in a few minutes (!)

1.7 The Parampool package

- Parampool[4] is a package for handling a large pool of input parameters in simulation programs
- Parampool can automatically create a sophisticated web-based graphical user interface (GUI) to set parameters and view solutions

Remark.

The forthcoming material aims at those with particular interest in equipping their programs with a GUI - others can safely skip it.

1.8 Making a compute function

- Key concept: a *compute function* that takes all input data as arguments and returning HTML code for viewing the results (e.g., plots and numbers)
- What we have: `decay_plot_mpl.py`[5]
- `main` function carries out simulations and plotting for a series of Δt values

[4] `https://github.com/hplgit/parampool`
[5] `http://tinyurl.com/jvzzcfn/decay/decay_plot_mpl.py`

- Goal: steer and view these experiments from a web GUI
- What to do:
  - create a compute function
  - call `parampool` functionality

The compute function `main_GUI`:

```
def main_GUI(I=1.0, a=.2, T=4.0,
         dt_values=[1.25, 0.75, 0.5, 0.1],
         theta_values=[0, 0.5, 1]):
```

1.9 The hard part of the compute function: the HTML code

- The results are to be displayed in a web page
- Only you know what to display in your problem
- Therefore, you need to specify the HTML code

Suppose `explore` solves the problem, makes a plot, computes the error *and* returns appropriate HTML code with the plot. Embed error and plots in a table:

```
def main_GUI(I=1.0, a=.2, T=4.0,
         dt_values=[1.25, 0.75, 0.5, 0.1],
         theta_values=[0, 0.5, 1]):
    # Build HTML code for web page. Arrange plots in columns
    # corresponding to the theta values, with dt down the rows
    theta2name = {0: 'FE', 1: 'BE', 0.5: 'CN'}
    html_text = '<table>\n'
    for dt in dt_values:
        html_text += '<tr>\n'
        for theta in theta_values:
            E, html = explore(I, a, T, dt, theta, makeplot=True)
            html_text += """
<td>
<center><b>%s, dt=%g, error: %s</b></center><br>
%s
</td>
""" % (theta2name[theta], dt, E, html)
        html_text += '</tr>\n'
    html_text += '</table>\n'
    return html_text
```

1.10 How to embed a PNG plot in HTML code

In `explore`:

```
import matplotlib.pyplot as plt
...
# plot
plt.plot(t, u, r-')
plt.xlabel('t')
plt.ylabel('u')
...
from parampool.utils import save_png_to_str
html_text = save_png_to_str(plt, plotwidth=400)
```

If you know HTML, you can return more sophisticated layout etc.

1.11 Generating the user interface

Make a file `decay_GUI_generate.py`:

```
from parampool.generator.flask import generate
from decay_GUI import main
generate(main,
         output_controller='decay_GUI_controller.py',
         output_template='decay_GUI_view.py',
         output_model='decay_GUI_model.py')
```

Running `decay_GUI_generate.py` results in

1. `decay_GUI_model.py` defines HTML widgets to be used to set input data in the web interface,
2. `templates/decay_GUI_views.py` defines the layout of the web page,
3. `decay_GUI_controller.py` runs the web application.

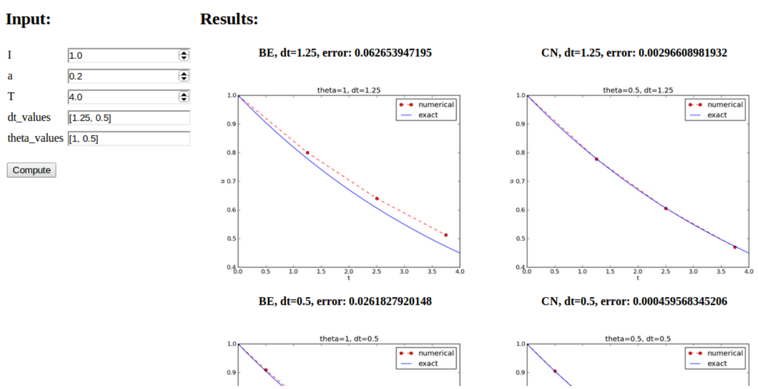
Good news: we only need to run `decay_GUI_controller.py` and there is no need to look into any of these files!

1.12 Running the web application

Start the GUI

```
Terminal> python decay_GUI_controller.py
```

Open a web browser at `127.0.0.1:5000`



1.13 More advanced use

- The compute function can have arguments of type float, int, string, list, dict, numpy array, filename (file upload)
- Alternative: specify a hierarchy of input parameters with name, default value, data type, widget type, unit (m, kg, s), validity check
- The generated web GUI can have user accounts with login and storage of results in a database

2 Computing convergence rates

Frequent assumption on the relation between the numerical error E and some discretization parameter Δt:

$$E = C\Delta t^r, \tag{1}$$

- Unknown: C and r.
- Goal: estimate r (and C) from numerical experiments

2.1 Estimating the convergence rate r

Perform numerical experiments: $(\Delta t_i, E_i)$, $i = 0, \ldots, m-1$. Two methods for finding r (and C):

1. Take the logarithm of (1), $\ln E = r\ln\Delta t + \ln C$, and fit a straight line to the data points $(\Delta t_i, E_i)$, $i = 0, \ldots, m-1$.
2. Consider two consecutive experiments, $(\Delta t_i, E_i)$ and $(\Delta t_{i-1}, E_{i-1})$. Dividing the equation $E_{i-1} = C\Delta t_{i-1}^r$ by $E_i = C\Delta t_i^r$ and solving for r yields

$$r_{i-1} = \frac{\ln(E_{i-1}/E_i)}{\ln(\Delta t_{i-1}/\Delta t_i)} \tag{2}$$

for $i = 1, = \ldots, m-1$.
Method 2 is best.

2.2 Implementation

Compute $r_0, r_1, \ldots, r_{m-2}$:

```
from math import log

def main():
    I, a, T, makeplot, dt_values = read_command_line()
    r = {}  # estimated convergence rates
    for theta in 0, 0.5, 1:
        E_values = []
        for dt in dt_values:
            E = explore(I, a, T, dt, theta, makeplot=False)
            E_values.append(E)
```

```
        # Compute convergence rates
        m = len(dt_values)
        r[theta] = [log(E_values[i-1]/E_values[i])/
                    log(dt_values[i-1]/dt_values[i])
                    for i in range(1, m, 1)]

    for theta in r:
        print '\nPairwise convergence rates for theta=%g:' % theta
        print ' '.join(['%.2f' % r_ for r_ in r[theta]])
    return r
```

Complete program: `decay_convrate.py`[6].

2.3 Execution

```
Terminal> python decay_convrate.py --dt 0.5 0.25 0.1 0.05 0.025 0.01
...
Pairwise convergence rates for theta=0:
1.33 1.15 1.07 1.03 1.02

Pairwise convergence rates for theta=0.5:
2.14 2.07 2.03 2.01 2.01

Pairwise convergence rates for theta=1:
0.98 0.99 0.99 1.00 1.00
```

Strong verification method.

Verify that r has the expected value!

2.4 Debugging via convergence rates

Potential bug: missing `a` in the denominator,

```
u[n+1] = (1 - (1-theta)*a*dt)/(1 + theta*dt)*u[n]
```

Running `decay_convrate.py` gives same rates.
Why? The value of a... ($a = 1$)
0 and 1 are *bad values* in tests!
Better:

```
Terminal> python decay_convrate.py --a 2.1 --I 0.1  \
          --dt 0.5 0.25 0.1 0.05 0.025 0.01
...
Pairwise convergence rates for theta=0:
1.49 1.18 1.07 1.04 1.02

Pairwise convergence rates for theta=0.5:
-1.42 -0.22 -0.07 -0.03 -0.01
```

[6]https://github.com/hplgit/INF5620/blob/gh-pages/src/decay/decay_convrate.py


```
Pairwise convergence rates for theta=1:
0.21 0.12 0.06 0.03 0.01
```

Forward Euler works...because $\theta = 0$ hides the bug.
This bug gives $r \approx 0$:

```
u[n+1] = ((1-theta)*a*dt)/(1 + theta*dt*a)*u[n]
```

3 Software engineering

Goal: make more professional numerical software.
Topics:

- How to make modules (reusable libraries)
- Testing frameworks (doctest, nose, unittest)
- Implementation with classes

3.1 Making a module

- Previous programs: much repetitive code (esp. `solver`)
- DRY (Don't Repeat Yourself) principle: no copies of code
- A change needs to be done in one *and only one* place
- Module = just a file with functions (reused through `import`)
- Let's make a module by putting these functions in a file:
  - `solver`
  - `verify_three_steps`
  - `verify_discrete_solution`
  - `explore`
  - `define_command_line_options`
  - `read_command_line`
  - `main` (with convergence rates)
  - `verify_convergence_rate`

Module name: `decay_mod`, filename: `decay_mod.py`.
Sketch:

```
from numpy import *
from matplotlib.pyplot import *
import sys

def solver(I, a, T, dt, theta):
    ...

def verify_three_steps():
    ...

def verify_exact_discrete_solution():
    ...

def u_exact(t, I, a):
    ...

def explore(I, a, T, dt, theta=0.5, makeplot=True):
    ...

def define_command_line_options():
    ...

def read_command_line(use_argparse=True):
    ...

def main():
    ...
```

That is! It's a module `decay_mod` in file `decay_mod.py`.

Usage in some other program:

```
from decay_mod import solver
u, t = solver(I=1.0, a=3.0, T=3, dt=0.01, theta=0.5)
```

3.2 Test block

At the end of a module it is common to include a *test block*:

```
if __name__ == '__main__':
    main()
```

- If `decay_mod` is imported, `__name__` is `decay_mod`.
- If `decay_mod.py` is run, `__name__` is `__main__`.
- Use test block for testing, demo, user interface, ...

Extended test block:

```
if __name__ == '__main__':
    if 'verify' in sys.argv:
        if verify_three_steps() and verify_discrete_solution():
            pass # ok
        else:
            print 'Bug in the implementation!'
    elif 'verify_rates' in sys.argv:
        sys.argv.remove('verify_rates')
        if not '--dt' in sys.argv:
            print 'Must assign several dt values'
```



```
            sys.exit(1)  # abort
        if verify_convergence_rate():
            pass
        else:
            print 'Bug in the implementation!'
    else:
        # Perform simulations
        main()
```

3.3 Prefixing imported functions by the module name

```
from numpy import *
from matplotlib.pyplot import *
```

This imports a large number of names (`sin`, `exp`, `linspace`, `plot`, ...).
Confusion: is a function from `numpy`? Or `matplotlib.pyplot`?
Alternative (recommended) import:

```
import numpy
import matplotlib.pyplot
```

Now we need to prefix functions with module name:

```
t = numpy.linspace(0, T, Nt+1)
u_e = I*numpy.exp(-a*t)
matplotlib.pyplot.plot(t, u_e)
```

Common standard:

```
import numpy as np
import matplotlib.pyplot as plt

t = np.linspace(0, T, Nt+1)
u_e = I*np.exp(-a*t)
plt.plot(t, u_e)
```

3.4 Downside of module prefix notation

A math line like $e^{-at}\sin(2\pi t)$ gets cluttered with module names,

```
numpy.exp(-a*t)*numpy.sin(2(numpy.pi*t)
# or
np.exp(-a*t)*np.sin(2*np.pi*t)
```

Solution (much used in this course): do two imports

```
import numpy as np
from numpy import exp, sin, pi
...
t = np.linspace(0, T, Nt+1)
u_e = exp(-a*t)*sin(2*pi*t)
```

3.5 Doctests

Doc strings can be equipped with interactive Python sessions for demonstrating usage and *automatic testing* of functions.

```
def solver(I, a, T, dt, theta):
    """
    Solve u'=-a*u, u(0)=I, for t in (0,T] with steps of dt.


    >>> u, t = solver(I=0.8, a=1.2, T=4, dt=0.5, theta=0.5)
    >>> for t_n, u_n in zip(t, u):
    ...     print 't=%.1f, u=%.14f' % (t_n, u_n)
    t=0.0, u=0.80000000000000
    t=0.5, u=0.43076923076923
    t=1.0, u=0.23195266272189
    t=1.5, u=0.12489758761948
    t=2.0, u=0.06725254717972
    t=2.5, u=0.03621291001985
    t=3.0, u=0.01949925924146
    t=3.5, u=0.01049960113002
    t=4.0, u=0.00565363137770
    """
    ...
```

3.6 Running doctests

Automatic check that the code reproduces the doctest output:

```
Terminal> python -m doctest decay_mod_doctest.py
```

Report in case of failure:

```
Terminal> python -m doctest decay_mod_doctest.py
********************************************************
File "decay_mod_doctest.py", line 12, in decay_mod_doctest....
Failed example:
    for t_n, u_n in zip(t, u):
        print 't=%.1f, u=%.14f' % (t_n, u_n)
Expected:
    t=0.0, u=0.80000000000000
    t=0.5, u=0.43076923076923
    t=1.0, u=0.23195266272189
    t=1.5, u=0.12489758761948
    t=2.0, u=0.06725254717972
Got:
    t=0.0, u=0.80000000000000
    t=0.5, u=0.43076923076923
    t=1.0, u=0.23195266272189
    t=1.5, u=0.12489758761948
    t=2.0, u=0.06725254718756
********************************************************
1 items had failures:
   1 of   2 in decay_mod_doctest.solver
***Test Failed*** 1 failures.
```


Floats are difficult to compare.

Limit the number of digits in the output in doctests! Otherwise, round-off errors on a different machine may ruin the test.

Complete program: `decay_mod_doctest.py`[7].

3.7 Unit testing with nose

- Nose is a very user-friendly testing framework
- Based on *unit testing*
- Identify (small) units of code and test each unit
- Nose automates running all tests
- Good habit: run all tests after (small) edits of a code
- Even better habit: write tests *before* the code (!)
- Remark: unit testing in scientific computing is not yet well established

3.8 Basic use of nose

1. Implement tests in *test functions* with names starting with `test_`.
2. Test functions cannot have arguments.
3. Test functions perform assertions on computed results using `assert` functions from the `nose.tools` module.
4. Test functions can be in the source code files or be collected in separate files `test*.py`.

3.9 Example on a nose test in the source code

Very simple module `mymod` (in file `mymod.py`):

```
def double(n):
    return 2*n
```

Write test function in `mymod.py`:

```
def double(n):
    return 2*n

import nose.tools as nt

def test_double():
    result = double(4)
    nt.assert_equal(result, 8)
```

Running

[7] http://tinyurl.com/jvzzcfn/decay/decay_mod_doctest.py

```
Terminal> nosetests -s mymod
```

makes the `nose` tool run all `test_*()` functions in `mymod.py`.

3.10 Example on a nose test in a separate file

Write the test in a separate file, say `test_mymod.py`:

```
import nose.tools as nt
import mymod

def test_double():
    result = mymod.double(4)
    nt.assert_equal(result, 8)
```

Running

```
Terminal> nosetests -s
```

makes the `nose` tool run all `test_*()` functions in all files `test*.py` in the current directory and in all subdirectories (recursevely) with names `tests` or `*_tests`.

Tip.

Start with test functions in the source code file. When the file contains many tests, or when you have many source code files, move tests to separate files.

3.11 The habit of writing nose tests

- Put `test_*()` functions in the module
- When you get many `test_*()` functions, collect them in `tests/test*.py`

3.12 Purpose of a test function: raise AssertionError if failure

Alternative ways of raising AssertionError if `result` is not 8:

```
import nose.tools as nt

def test_double():
    result = ...

    nt.assert_equal(result, 8)    # alternative 1

    assert result == 8            # alternative 2

    if result != 8:               # alternative 3
        raise AssertionError()
```


3.13 Advantages of nose

- Easier to use than other test frameworks
- Tests are written and collected in a *compact* and structured way
- Large collections of tests, scattered throughout a directory tree can be executed with one command (`nosetests -s`)
- Nose is a much-adopted standard

3.14 Demonstrating nose (ideas)

Aim: test function `solver` for $u' = -au$, $u(0) = I$.

We design three unit tests:

1. A comparison between the computed u^n values and the exact discrete solution
2. A comparison between the computed u^n values and precomputed verified reference values
3. A comparison between observed and expected convergence rates

These tests follow very closely the previous `verify*` functions.

3.15 Demonstrating nose (code)

```
import nose.tools as nt
import decay_mod_unittest as decay_mod
import numpy as np

def exact_discrete_solution(n, I, a, theta, dt):
    """Return exact discrete solution of the theta scheme."""
    dt = float(dt)  # avoid integer division
    factor = (1 - (1-theta)*a*dt)/(1 + theta*dt*a)
    return I*factor**n

def test_exact_discrete_solution():
    """
    Compare result from solver against
    formula for the discrete solution.
    """
    theta = 0.8; a = 2; I = 0.1; dt = 0.8
    N = int(8/dt)  # no of steps
    u, t = decay_mod.solver(I=I, a=a, T=N*dt, dt=dt, theta=theta)
    u_de = np.array([exact_discrete_solution(n, I, a, theta, dt)
                     for n in range(N+1)])
    diff = np.abs(u_de - u).max()
    nt.assert_almost_equal(diff, 0, delta=1E-14)
```

3.16 Floats as test results require careful comparison

- Round-off errors make exact comparison of floats unreliable
- `nt.assert_almost_equal`: compare two floats to some digits or precision

```
def test_solver():
    """
    Compare result from solver against
    precomputed arrays for theta=0, 0.5, 1.
    """
    I=0.8; a=1.2; T=4; dt=0.5  # fixed parameters
    precomputed = {
        't': np.array([ 0. ,  0.5,  1. ,  1.5,  2. ,  2.5,
                        3. ,  3.5,  4. ]),
        0.5: np.array(
            [ 0.8       ,  0.43076923,  0.23195266, 0.12489759,
              0.06725255,  0.03621291,  0.01949926, 0.0104996 ,
              0.00565363]),
        0: ...,
        1: ...
        }
    for theta in 0, 0.5, 1:
        u, t = decay_mod.solver(I, a, T, dt, theta=theta)
        diff = np.abs(u - precomputed[theta]).max()
        # Precomputed numbers are known to 8 decimal places
        nt.assert_almost_equal(diff, 0, places=8,
                               msg='theta=%s' % theta)
```

3.17 Test of wrong use

- Find input data that may cause trouble and test such cases
- Here: the formula for u^{n+1} may involve integer division

Example:

```
theta = 1; a = 1; I = 1; dt = 2
```

may lead to integer division:

```
(1 - (1-theta)*a*dt)  # becomes 1
(1 + theta*dt*a)      # becomes 2
(1 - (1-theta)*a*dt)/(1 + theta*dt*a)  # becomes 0 (!)
```

Test that `solver` does not suffer from such integer division:

```
def test_potential_integer_division():
    """Choose variables that can trigger integer division."""
    theta = 1; a = 1; I = 1; dt = 2
    N = 4
    u, t = decay_mod.solver(I=I, a=a, T=N*dt, dt=dt, theta=theta)
    u_de = np.array([exact_discrete_solution(n, I, a, theta, dt)
                     for n in range(N+1)])
    diff = np.abs(u_de - u).max()
    nt.assert_almost_equal(diff, 0, delta=1E-14)
```

3.18 Test of convergence rates

Convergence rate tests are very common for differential equation solvers.


```
def test_convergence_rates():
    """Compare empirical convergence rates to exact ones."""
    # Set command-line arguments directly in sys.argv
    import sys
    sys.argv[1:] = '--I 0.8 --a 2.1 --T 5 '\
                   '--dt 0.4 0.2 0.1 0.05 0.025'.split()
    r = decay_mod.main()
    for theta in r:
        nt.assert_true(r[theta])  # check for non-empty list

    expected_rates = {0: 1, 1: 1, 0.5: 2}
    for theta in r:
        r_final = r[theta][-1]
        # Compare to 1 decimal place
        nt.assert_almost_equal(expected_rates[theta], r_final,
                               places=1, msg='theta=%s' % theta)
```

Complete program: `test_decay_nose.py`[8].

3.19 Classical unit testing with unittest

- `unittest` is a Python module mimicing the classical JUnit class-based unit testing framework from Java
- This is how unit testing is normally done
- Requires knowledge of object-oriented programming

Remark.

You will probably not use it, but you're not educated unless you know what unit testing with classes is.

3.20 Basic use of unittest

Write file `test_mymod.py`:

```
import unittest
import mymod

class TestMyCode(unittest.TestCase):
    def test_double(self):
        result = mymod.double(4)
        self.assertEqual(result, 8)

if __name__ == '__main__':
    unittest.main()
```

3.21 Demonstration of unittest

[8] http://tinyurl.com/jvzzcfn/decay/tests/test_decay_nose.py

```
import unittest
import decay_mod_unittest as decay
import numpy as np

def exact_discrete_solution(n, I, a, theta, dt):
    factor = (1 - (1-theta)*a*dt)/(1 + theta*dt*a)
    return I*factor**n

class TestDecay(unittest.TestCase):

    def test_exact_discrete_solution(self):
        ...
        diff = np.abs(u_de - u).max()
        self.assertAlmostEqual(diff, 0, delta=1E-14)

    def test_solver(self):
        ...
        for theta in 0, 0.5, 1:
            ...
            self.assertAlmostEqual(diff, 0, places=8,
                                   msg='theta=%s' % theta)

    def test_potential_integer_division():
        ...
        self.assertAlmostEqual(diff, 0, delta=1E-14)

    def test_convergence_rates(self):
        ...
        for theta in r:
            ...
            self.assertAlmostEqual(...)

if __name__ == '__main__':
    unittest.main()
```

Complete program: `test_decay_unittest.py`[9].

4 Implementing simple problem and solver classes

- So far: programs are built of Python functions
- New focus: alternative implementations using classes
- Class-based implementations are very popular, especially in business/adm applications
- Class-based implementations scales better to large and complex scientific applications

4.1 What to learn

Tasks:

- Explain basic use of classes to build a differential equation solver
- Introduce concepts that make such programs easily scale to more complex applications
- Demonstrate the advantage of using classes

[9] `http://tinyurl.com/jvzzcfn/decay/tests/test_decay_nose.py`

Ideas:

- Classes for Problem, Solver, and Visualizer
- Problem: all the physics information about the problem
- Solver: all the numerics information + numerical computations
- Visualizer: plot the solution and other quantities

4.2 The problem class

- Model problem: $u' = -au$, $u(0) = I$, for $t \in (0, T]$.
- Class `Problem` stores the physical parameters a, I, T
- May also offer other data, e.g., $u_e(t) = Ie^{-at}$

Implementation:

```
from numpy import exp

class Problem:
    def __init__(self, I=1, a=1, T=10):
        self.T, self.I, self.a = I, float(a), T

    def u_exact(self, t):
        I, a = self.I, self.a     # extract local variables
        return I*exp(-a*t)
```

Basic usage:

```
problem = Problem(T=5)
problem.T = 8
problem.dt = 1.5
```

4.3 Improved problem class

More flexible input from the command line:

```
class Problem:
    def __init__(self, I=1, a=1, T=10):
        self.T, self.I, self.a = I, float(a), T

    def define_command_line_options(self, parser=None):
        if parser is None:
            import argparse
            parser = argparse.ArgumentParser()

        parser.add_argument(
            '--I', '--initial_condition', type=float,
            default=self.I, help='initial condition, u(0)',
            metavar='I')
        parser.add_argument(
            '--a', type=float, default=self.a,
            help='coefficient in ODE', metavar='a')
        parser.add_argument(
```

```
            '--T', '--stop_time', type=float, default=self.T,
            help='end time of simulation', metavar='T')
        return parser

    def init_from_command_line(self, args):
        self.I, self.a, self.T = args.I, args.a, args.T

    def exact_solution(self, t):
        I, a = self.I, self.a
        return I*exp(-a*t)
```

- Can utilize user's `ArgumentParser`, or make one
- `None` is used to indicate a non-initialized variable

4.4 The solver class

- Store numerical data Δt, θ
- Compute solution and quantities derived from the solution

Implementation:

```
class Solver:
    def __init__(self, problem, dt=0.1, theta=0.5):
        self.problem = problem
        self.dt, self.theta = float(dt), theta

    def define_command_line_options(self, parser):
        parser.add_argument(
            '--dt', '--time_step_value', type=float,
            default=0.5, help='time step value', metavar='dt')
        parser.add_argument(
            '--theta', type=float, default=0.5,
            help='time discretization parameter', metavar='dt')
        return parser

    def init_from_command_line(self, args):
        self.dt, self.theta = args.dt, args.theta

    def solve(self):
        from decay_mod import solver
        self.u, self.t = solver(
            self.problem.I, self.problem.a, self.problem.T,
            self.dt, self.theta)
```

Note: reuse of the numerical algorithm from the `decay_mod` module (i.e., the class is a wrapper of the procedural implementation).

4.5 The visualizer class

```
class Visualizer:
    def __init__(self, problem, solver):
        self.problem, self.solver = problem, solver

    def plot(self, include_exact=True, plt=None):
        """
```



```
        Add solver.u curve to the plotting object plt,
        and include the exact solution if include_exact is True.
        This plot function can be called several times (if
        the solver object has computed new solutions).
        """
        if plt is None:
            import scitools.std  as plt # can use matplotlib as well

        plt.plot(self.solver.t, self.solver.u, '--o')
        plt.hold('on')
        theta2name = {0: 'FE', 1: 'BE', 0.5: 'CN'}
        name = theta2name.get(self.solver.theta, '')
        legends = ['numerical %s' % name]
        if include_exact:
            t_e = linspace(0, self.problem.T, 1001)
            u_e = self.problem.exact_solution(t_e)
            plt.plot(t_e, u_e, 'b-')
            legends.append('exact')
        plt.legend(legends)
        plt.xlabel('t')
        plt.ylabel('u')
        plt.title('theta=%g, dt=%g' %
                  (self.solver.theta, self.solver.dt))
        plt.savefig('%s_%g.png' % (name, self.solver.dt))
        return plt
```

Remark: The `plt` object in `plot` adds a new curve to a plot, which enables comparing different solutions from different runs of `Solver.solve`

4.6 Combing the classes

Let `Problem`, `Solver`, and `Visualizer` play together:

```
def main():
    problem = Problem()
    solver = Solver(problem)
    viz = Visualizer(problem, solver)

    # Read input from the command line
    parser = problem.define_command_line_options()
    parser = solver. define_command_line_options(parser)
    args = parser.parse_args()
    problem.init_from_command_line(args)
    solver. init_from_command_line(args)

    # Solve and plot
    solver.solve()
    import matplotlib.pyplot as plt
    #import scitools.std as plt
    plt = viz.plot(plt=plt)
    E = solver.error()
    if E is not None:
        print 'Error: %.4E' % E
    plt.show()
```

Complete program: `decay_class.py`[10].

[10] http://tinyurl.com/jvzzcfn/decay/decay_class.py

5 Implementing more advanced problem and solver classes

- The previous `Problem` and `Solver` classes soon contain much repetitive code when the number of parameters increases
- Much of such code can be parameterized and be made more compact
- Idea: collect all parameters in a dictionary `self.prms`, with two associated dictionaries `self.types` and `self.help` for holding associated object types and help strings
- Collect common code in class `Parameters`
- Let `Problem`, `Solver`, and maybe `Visualizer` be subclasses of class `Parameters`, basically defining `self.prms`, `self.types`, `self.help`

5.1 A generic class for parameters

```
class Parameters:
    def set(self, **parameters):
        for name in parameters:
            self.prms[name] = parameters[name]

    def get(self, name):
        return self.prms[name]

    def define_command_line_options(self, parser=None):
        if parser is None:
            import argparse
            parser = argparse.ArgumentParser()

        for name in self.prms:
            tp = self.types[name] if name in self.types else str
            help = self.help[name] if name in self.help else None
            parser.add_argument(
                '--' + name, default=self.get(name), metavar=name,
                type=tp, help=help)

        return parser

    def init_from_command_line(self, args):
        for name in self.prms:
            self.prms[name] = getattr(args, name)
```

Slightly more advanced version in `class_decay_verf1.py`[11].

5.2 The problem class

```
class Problem(Parameters):
    """
    Physical parameters for the problem u'=-a*u, u(0)=I,
    with t in [0,T].
    """
    def __init__(self):
        self.prms = dict(I=1, a=1, T=10)
        self.types = dict(I=float, a=float, T=float)
```

[11] http://tinyurl.com/jvzzcfn/decay/class_decay_verf1.py


```
        self.help = dict(I='initial condition, u(0)',
                         a='coefficient in ODE',
                         T='end time of simulation')

    def exact_solution(self, t):
        I, a = self.get('I'), self.get('a')
        return I*np.exp(-a*t)
```

5.3 The solver class

```
class Solver(Parameters):
    def __init__(self, problem):
        self.problem = problem
        self.prms = dict(dt=0.5, theta=0.5)
        self.types = dict(dt=float, theta=float)
        self.help = dict(dt='time step value',
                         theta='time discretization parameter')

    def solve(self):
        from decay_mod import solver
        self.u, self.t = solver(
            self.problem.get('I'),
            self.problem.get('a'),
            self.problem.get('T'),
            self.get('dt'),
            self.get('theta'))

    def error(self):
        try:
            u_e = self.problem.exact_solution(self.t)
            e = u_e - self.u
            E = np.sqrt(self.get('dt')*np.sum(e**2))
        except AttributeError:
            E = None
        return E
```

5.4 The visualizer class

- No parameters needed (for this simple problem), no need to inherit class `Parameters`
- Same code as previously shown class `Visualizer`
- Same code as previously shown for combining `Problem`, `Solver`, and `Visualizer`

6 Performing scientific experiments

Goal: explore the behavior of a numerical method for a differential equation and show how scientific experiments can be set up and reported.

Tasks:

- Write scripts to automate experiments
- Generate scientific reports from scripts

Tools to learn:

- `os.system` for running other programs
- `subprocess` for running other programs and extracting the output
- List comprehensions
- Formats for scientific reports: HTML w/MathJax, LaTeX, Sphinx, DocOnce

6.1 Model problem and numerical solution method

Problem:

$$u'(t) = -au(t), \quad u(0) = I,\ 0 < t \le T, \tag{3}$$

Solution method (θ-rule):

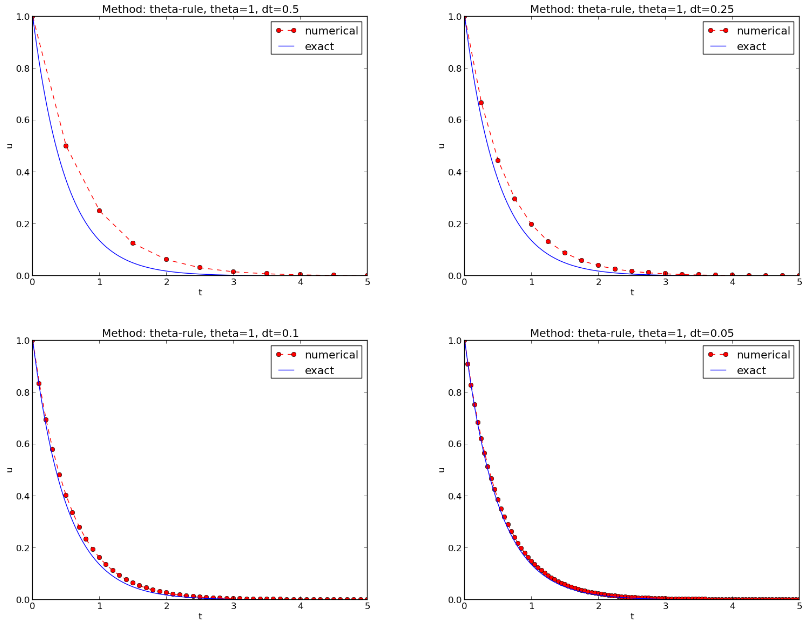
$$u^{n+1} = \frac{1 - (1-\theta)a\Delta t}{1 + \theta a\Delta t}u^n, \quad u^0 = I\,.$$

6.2 Plan for the experiments

- Plot u^n against $u_{\mathrm{e}} = Ie^{-at}$ for various choices of the parameters I, a, Δt, and θ
- How does the discrete solution compare with the exact solution when Δt is varied and $\theta = 0, 0.5, 1$?
- Use the `decay_mod.py`[12] module (little modification of the plotting, see `experiments/decay_mod.py`[13])
- Make separate program for running (automating) the experiments (*script*)
  1. `python decay_mod.py --I 1 --a 2 --makeplot --T 5 --dt 0.5 0.25 0.1 0.05`
  2. Combine generated figures `FE_*.png`, `BE_*.png`, and `CN_*.png` to new figures with multiple plots
  3. Run script as `python decay_exper0.py 0.5 0.25 0.1 0.05` (Δt values on the command line)

[12] `http://tinyurl.com/jvzzcfn/decay/decay_mod.py`
[13] `http://tinyurl.com/jvzzcfn/decay/experiments/decay_mod.py`

6.3 Typical plot summarizing the results



6.4 Script code

Typical *script* (small administering program) for running the experiments:

```
import os, sys

def run_experiments(I=1, a=2, T=5):
    # The command line must contain dt values
    if len(sys.argv) > 1:
        dt_values = [float(arg) for arg in sys.argv[1:]]
    else:
        print 'Usage: %s dt1 dt2 dt3 ...' %  sys.argv[0]
        sys.exit(1)  # abort

    # Run module file as a stand-alone application
    cmd = 'python decay_mod.py --I %g --a %g --makeplot --T %g' % \
          (I, a, T)
    dt_values_str = ' '.join([str(v) for v in dt_values])
    cmd += ' --dt %s' % dt_values_str
    print cmd
    failure = os.system(cmd)
```

```
    if failure:
        print 'Command failed:', cmd; sys.exit(1)

    # Combine images into rows with 2 plots in each row
    image_commands = []
    for method in 'BE', 'CN', 'FE':
        pdf_files = ' '.join(['%s_%g.pdf' % (method, dt)
                              for dt in dt_values])
        png_files = ' '.join(['%s_%g.png' % (method, dt)
                              for dt in dt_values])
        image_commands.append(
            'montage -background white -geometry 100%' +
            ' -tile 2x %s %s.png' % (png_files, method))
        image_commands.append(
            'convert -trim %s.png %s.png' % (method, method))
        image_commands.append(
            'convert %s.png -transparent white %s.png' %
            (method, method))
        image_commands.append(
            'pdftk %s output tmp.pdf' % pdf_files)
        num_rows = int(round(len(dt_values)/2.0))
        image_commands.append(
            'pdfnup --nup 2x%d tmp.pdf' % num_rows)
        image_commands.append(
            'pdfcrop tmp-nup.pdf %s.pdf' % method)

    for cmd in image_commands:
        print cmd
        failure = os.system(cmd)
        if failure:
            print 'Command failed:', cmd; sys.exit(1)

    # Remove the files generated above and by decay_mod.py
    from glob import glob
    filenames = glob('*_*.png') + glob('*_*.pdf') + \
                glob('*_*.eps') + glob('tmp*.pdf')
    for filename in filenames:
        os.remove(filename)

if __name__ == '__main__':
    run_experiments()
```

Complete program: `experiments/decay_exper0.py`[14].

6.5 Comments to the code

Many useful constructs in the previous script:

- `[float(arg) for arg in sys.argv[1:]]` builds a list of real numbers from all the command-line arguments
- `failure = os.system(cmd)` runs an operating system command (e.g., another program)
- `sys.exit(1)` aborts the program
- `['%s_%s.png' % (method, dt) for dt in dt_values]` builds a list of filenames from a list of numbers (`dt_values`)
- All `montage` commands for creating composite figures are stored in a list and thereafter executed in a loop

[14] http://tinyurl.com/jvzzcfn/decay/experiments/decay_exper0.py

- `glob.glob('*_*.png')` returns a list of the names of all files in the current folder where the filename matches the *Unix wildcard notation* `*_*.png` (meaning "any text, underscore, any text, and then '.png'")
- `os.remove(filename)` removes the file with name `filename`

6.6 Interpreting output from other programs

In `decay_exper0.py` we run a program (`os.system`) and want to grab the output, e.g.,

```
Terminal> python decay_plot_mpl.py
0.0   0.40:    2.105E-01
0.0   0.04:    1.449E-02
0.5   0.40:    3.362E-02
0.5   0.04:    1.887E-04
1.0   0.40:    1.030E-01
1.0   0.04:    1.382E-02
```

Tasks:

- read the output from the `decay_mod.py` program
- interpret this output and store the E values in arrays for each θ value
- plot E versus Δt, for each θ, in a log-log plot

6.7 Code for grabbing output from another program

Use the `subprocess` module to grab output:

```
from subprocess import Popen, PIPE, STDOUT
p = Popen(cmd, shell=True, stdout=PIPE, stderr=STDOUT)
output, dummy = p.communicate()
failure = p.returncode
if failure:
    print 'Command failed:', cmd; sys.exit(1)
```

6.8 Code for interpreting the grabbed output

- Run through the `output` string, line by line
- If the current line prints θ, Δt, and E, split the line into these three pieces and store the data
- Store data in a dictionary `errors` with keys `dt` and the three θ values

```
errors = {'dt': dt_values, 1: [], 0: [], 0.5: []}
for line in output.splitlines():
    words = line.split()
    if words[0] in ('0.0', '0.5', '1.0'):  # line with E?
        # typical line: 0.0   1.25:    7.463E+00
        theta = float(words[0])
        E = float(words[2])
        errors[theta].append(E)
```

Next: plot E versus Δt for $\theta = 0, 0.5, 1$
Complete program: `experiments/decay_exper1.py`[15]. Fine recipe for

- how to run other programs
- how to extract and interpret output from other programs
- how to automate many manual steps in creating simulations and figures

6.9 Making a report

- Scientific investigations are best documented in a report!
- A sample report[16]
- How can we write such a report?
- First problem: what format should I write in?
- Plain HTML[17], generated by `decay_exper1_html.py`[18]
- HTML with MathJax[19], generated by `decay_exper1_mathjax.py`[20]
- LaTeX PDF[21], based on LaTeX source[22]
- Sphinx HTML[23], based on reStructuredText[24]
- Markdown, MediaWiki, ...
- DocOnce[25] can generate LaTeX, HTML w/MathJax, Sphinx, Markdown, MediaWiki, ... (DocOnce source[26] for the examples above, and Python program for generating the DocOnce source[27])
- Examples on different report formats[28]

[15] http://tinyurl.com/jvzzcfn/decay/experiments/decay_exper1.py
[16] http://hplgit.github.com/INF5620/doc/writing_reports/sphinx-cloud/
[17] http://hplgit.github.com/INF5620/doc/writing_reports/report_html.html
[18] http://tinyurl.com/jvzzcfn/decay/experiments/decay_exper1_html.py
[19] http://hplgit.github.com/INF5620/doc/writing_reports/report_html_mathjax.html
[20] http://tinyurl.com/jvzzcfn/decay/experiments/decay_exper1_html.py
[21] http://hplgit.github.com/INF5620/doc/writing_reports/report.pdf
[22] http://hplgit.github.com/INF5620/doc/writing_reports/report.tex.html
[23] http://hplgit.github.com/INF5620/doc/writing_reports/sphinx-cloud/index.html
[24] http://hplgit.github.com/INF5620/doc/writing_reports/report_sphinx.rst.html
[25] https://github.com/hplgit/doconce
[26] http://hplgit.github.com/INF5620/doc/writing_reports/report.do.txt.html
[27] http://tinyurl.com/jvzzcfn/decay/experiments/decay_exper1_do.py
[28] http://hplgit.github.com/INF5620/doc/writing_reports/

6.10 Publishing a complete project

- Make folder (directory) tree
- Keep track of all files via a *version control system* (Mercurial, Git, ...)
- Publish as private or public repository
- Utilize Bitbucket, Googlecode, GitHub, or similar
- See the intro to such tools[29]

[29] http://hplgit.github.com/teamods/bitgit/html/

Index