AMath 483/583 — Lecture 27 — May 27, 2011

Today:

- Python exception handling
- Python plus Fortran: f2py

Next week:

- More Python plus Fortran
- Visualization
- Parallel IPython

Read: Class notes and references

Exceptions in Python

If you try to do something illegal in Python it will generally raise an exception.

```
>>> x = 0.
>>> y = 1/x
Traceback (most recent call last):
ZeroDivisionError: float division
```

The exception ZeroDivisionError was raised when we tried to divide by 0.

```
>>> x = "8.0"
>>> y = 1/x
Traceback (most recent call last):
TypeError: unsupported operand type(s)
for /: 'int' and 'str'
```

The exception TypeError is raised if we try to divide by a string.

Exceptions in Python

Trying to access a variable not yet set gives:

```
>>> z = z+1
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
NameError: name 'z' is not defined
```

If this happens in a longer program, the program will die. Suppose that if z is not yet defined we want to set z=0 instead of incrementing it. Then we could use:

```
>>> try:
...     z = z+1
... except:
...     z = 0
...
>>> z
0
```


Exceptions in Python

You can specify different behavior for different exceptions:

```
x = 0.
try:
    y = 1/x
except ZeroDivisionError:
    print "Can't divide by 0!"
except TypeError:
    print "Can't divide by ",type(x)
```

produces:

```
Can't divide by 0!
```

Exceptions in Python

From `$CLASSHG/codes/python/plotheat2d.py`:

```
x, y, u = np.loadtxt('heatsoln.txt', unpack=True)

# Solution is plotted on n by n grid so length of
# each vector should be n**2
# Determine n:
try:
    n = int(np.sqrt(len(x)))
except:
    print "Expected len(x) to be a perfect square,
          "len(x) = ",len(x)
    raise ValueError

X = x.reshape(n,n)
Y = y.reshape(n,n)
U = u.reshape(n,n)
```


Exceptions in Python

Even better:

```
try:
    fname = 'heatsoln.txt'
    x, y, u = np.loadtxt(fname, unpack=True)
except:
    err_msg = "Could not load data from file %s" \
              % fname \
              + " Did you forget to run the program?"
    raise Exception(err_msg)
```


Exceptions in Python

This gives:

```
In [58]: run plotheat2d.py
---------------------------------------------------------
Exception                                 Traceback (mos

/Users/rjl/hg/uwamath583s11/codes/python/plotheat2d.py i
     11     err_msg = "Could not load data from file %s.
     12               + " Did you forget to run the prog
---> 13     raise Exception(err_msg)
     14
     15

Exception: Could not load data from file heatsoln.txt.
Did you forget to run the program?
WARNING: Failure executing file: <plotheat2d.py>
```


NumPy Inf and NaN

Note: Division by zero in NumPy arrays may be allowed, results in special values (NaN = Not a Number):

```
>>> x = np.linspace(-2.,2.,5)
>>> x
array([-2., -1.,  0.,  1.,  2.])

>>> x/0.
array([-Inf, -Inf,  NaN,  Inf,  Inf])
```

This is useful because often only a few values are "bad".
Note — can set to raise these exceptions:

```
>>> oldsettings = np.seterr(all = 'raise')
```

To set back to ignoring them:

```
>>> oldsettings = np.seterr(all = 'ignore')
```

Not-a-Number (NaN)

Some arithmetic operations give undefined results.

The result of such an operation is often replaced by a special value representing NaN.

Examples:

$0/0 =$ NaN

$0*$Infinity$=$ NaN

Using exceptions in NumPy

Suppose we want to evaluate $y_i = \sin(x_i)/x_i$ at many points.

If $x_i = 0$, must use l'Hôpital's rule: $\lim_{x\to 0} \frac{\sin(x)}{x} = 1$

Could program with a loop (very slow in Python!)

```
x = np.linspace(-10, 10, 100001)
y = np.ones(x.shape)

for i,xi in enumerate(x):
    if xi !=0:
        y[i] = np.sin(xi) / xi
```

Takes about 0.94 seconds

Can time using `time.clock() function`.
See `$CLASSHG/codes/python/timing1.py`.

Using exceptions in NumPy

Better solution: (no loop)

```
# ignore floating point exceptions:
oldsettings = np.seterr(all='ignore')

z = np.sin(x) / x          # contains a NaN

y = np.where(x != 0, z, 1.)
# sets y[i] = z[j] where x[j] != 0.
#           = 1.   where x[j] == 0.
```

Takes about 0.011 seconds.

Uses vectorized operation.

Python tools for debugging

- unittest module,
- assert statements: raise an Exception if what's asserted is not actually true,
- pdb, Python debugger
- Integrated Development Environments (IDEs), e.g. IDLE, Eclipse, Emacs

Demo... See also: Python Debugging section of the notes

f2py — combining Fortran and Python

Often want to use
- Fortran for intensive computations,
- Python to provide nice user interface, plot results,
  - automate a series of runs with different parameters,
  - do convergence tests as grid size is refined, etc.

Can write data files to disk from Fortran, read into Python,
- This is what we've done for plotting in homeworks.

Sometimes nice to call Fortran directly from Python.
- e.g. LAPACK is used under the hood in NumPy.

f2py provides a wrapper for Fortran code.

f2py — combining Fortran and Python

Basic idea:

`fortrancode.f90` contains a function or subroutine, e.g.
- function `f1(x)` that returns a single value.

```
$ f2py -m mymodulename -c fortrancode.f90
```

This creates a binary file `mymodulename.so` that can used as a Python module.

```
>>> from mymodulename import f1
>>> y = f1(3.)
```


f2py — function example

`$CLASSHG/codes/f2py/fcn1.f90`

```
function f1(x)
    real(kind=8), intent(in) :: x
    real(kind=8) :: f1
    f1 = exp(x)
end function f1
```

Then we can do...

```
$ f2py -m fcn1 -c fcn1.f90
$ python
>>> import fcn1
>>> fcn1.f1(1.)
2.7182818284590451
```


f2py — subroutine example

`$CLASSHG/codes/f2py/sub1.f90`

```
subroutine mysub(a,b,c,d)
    real (kind=8), intent(in) :: a,b
    real (kind=8), intent(out) :: c,d
    c = a+b
    d = a-b
end subroutine mysub
```

Then we can do...

```
$ f2py -m sub1 -c sub1.f90
$ python
>>> import sub1
>>> y = sub1.mysub(3., 5.)
>>> print y
(8.0, -2.0)
```

Note: Tuple `(c, d)` is returned by the Python function.

f2py — Jacobi iteration

`$CLASSHG/codes/f2py/jacobi1.f90`

```
    subroutine iterate(u0,iters,f,u,n)
```

Takes input array `u0` of length `n` and right hand side array `f` and produces `u` by taking `iters` iterations of Jacobi.

`$CLASSHG/codes/f2py/plot_jacobi_iterates.py`

```
    # Set u = initial guess;  f = rhs
    for nn in range(nplots):
        u = jacobi1.iterate(u, iters_per_plot, f)
        plt.plot(x, u, 'o-')
        plt.draw()
        time.sleep(.5)
```


Other wrappers...

- fwrap: Improved version of f2py coming soon.
  Wraps Fortran in C, Cython, Python.
  http://fortrancython.wordpress.com/
- swig: Connects C and C++ to many other languages
  http://www.swig.org/
- Cython: Allows writing C code embedded in Python.
  http://www.cython.org/
- Jython: For Java.
  http://www.jython.org/