Ch.3: Functions and branching

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We have used many Python functions

Mathematical functions:

```
from math import *
y = sin(x)*log(x)
```

Other functions:

```
n = len(somelist)
ints = range(5, n, 2)
```

Functions used with the dot syntax (called *methods*):

```
C = [5, 10, 40, 45]
i = C.index(10)        # result: i=1
C.append(50)
C.insert(2, 20)
```

What is a function? So far we have seen that we put some objects in and sometimes get an object (result) out of functions. Now it is time to write our own functions!

Python functions

- Function = a collection of statements we can execute wherever and whenever we want
- Function can take input objects and produce output objects
- Functions help to organize programs, make them more understandable, shorter, and easier to extend

Simple example: a mathematical function $F(C) = \frac{9}{5}C + 32$

```
def F(C):
    return (9.0/5)*C + 32
```

Note:

- Functions start with `def`, then the name of the function, then a list of arguments (here `C`) - the *function header*
- Inside the function: statements - the *function body*
- Wherever we want, inside the function, we can "stop the function" and return as many values/variables we want

Functions must be called

- A function does not do anything before it is called

```
a = 10
F1 = F(a)                                   # call
temp = F(15.5)                              # call
print F(a+1)                                # call
sum_temp = F(10) + F(20)                    # two calls
Fdegrees = [F(C) for C in Cdegrees]         # multiple calls
```

Note: Since `F(C)` produces (returns) a `float` object, we can call `F(C)` everywhere a `float` can be used

Local variables in Functions

Example: sum the integers from `start` to `stop`

```
def sumint(start, stop):
    s = 0      # variable for accumulating the sum
    i = start  # counter
    while i <= stop:
        s += i
        i += 1
    return s

print sumint(0, 10)
sum_10_100 = sumint(10, 100)
```

Note:

- `i` and `s` are local variables in `sumint` - these are destroyed at the end (return) of the function and never visible outside the function (in the calling program); in fact, `start` and `stop` are also local variables
- There is one global variable: `sum_10_100`, visible everywhere
- Read Chapter 3.1.3 in the book about local and global variables!

Turn a formula into a Python function

Formula: $y(t) = v_0t - \frac{1}{2}gt^2$. Make a Python function of it:

```
def yfunc(t, v0):
    g = 9.81
    return v0*t - 0.5*g*t**2

# sample calls:
y = yfunc(0.1, 6)
y = yfunc(0.1, v0=6)
y = yfunc(t=0.1, v0=6)
y = yfunc(v0=6, t=0.1)
```

Functions can have as many arguments as you like.

Function arguments become local variables

```python
def yfunc(t, v0):
    g = 9.81
    return v0*t - 0.5*g*t**2
```

When calling `yfunc(0.1, 6)`, all these statements are in fact executed:

```python
t = 0.1  # arguments get values as in standard assignments
v0 = 6
g = 9.81
return v0*t - 0.5*g*t**2
# local variables t, v0, g are destroyed
```

Functions may access global variables

The `y(t,v0)` function took two arguments. Could implement $y(t)$ as a function of t only:

```python
>>> def yfunc(t):
...     g = 9.81
...     return v0*t - 0.5*g*t**2
...
>>> yfunc(0.6)
...
NameError: global name 'v0' is not defined
```

Problem: `v0` must be defined in the calling program program before we call `yfunc`

```python
>>> v0 = 5
>>> yfunc(0.6)
1.2342
```

Note:

- `v0` is a global variable
- Global variables are variables defined outside functions
- Global variables are visible everywhere in a program

Functions can return multiple values

Say we want to compute $y(t)$ and $y'(t) = v_0 - gt$:

```python
def yfunc(t, v0):
    g = 9.81
    y = v0*t - 0.5*g*t**2
    dydt = v0 - g*t
    return y, dydt

# call:
position, velocity = yfunc(0.6, 3)
```

Separate the objects to be returned by comma, assign to variables separated by comma. Actually, a tuple is returned:

```python
>>> def f(x):
...     return x, x**2, x**4
...
>>> s = f(2)
>>> s
(2, 4, 16)
>>> type(s)
<type 'tuple'>
>>> x, x2, x4 = f(2)
```

Example: Compute a function defined as a sum

The function

$$L(x;n) = \sum_{i=1}^{n} \frac{1}{i}\left(\frac{x}{1+x}\right)^i$$

is an approximation to $\ln(1+x)$ for a finite n and $x \geq 1$.
Make a Python function for $L(x;n)$:

```python
def L(x, n):
    x = float(x)  # ensure float division below
    s = 0
    for i in range(1, n+1):
        s += (1.0/i)*(x/(1+x))**i
    return s

x = 5
from math import log as ln
print L(x, 10), L(x, 100), ln(1+x)
```

Returning errors as well from the L(x, n) function

We can return more: also the first neglected term in the sum and the error ($\ln(1+x) - L(x;n)$):

```python
def L2(x, n):
    x = float(x)
    s = 0
    for i in range(1, n+1):
        s += (1.0/i)*(x/(1+x))**i
    value_of_sum = s
    first_neglected_term = (1.0/(n+1))*(x/(1+x))**(n+1)
    from math import log
    exact_error = log(1+x) - value_of_sum
    return value_of_sum, first_neglected_term, exact_error

# typical call:
x = 1.2; n = 100
value, approximate_error, exact_error = L2(x, n)
```

Functions do not need to return objects

```python
def somefunc(obj):
    print obj

return_value = somefunc(3.4)
```

Here, `return_value` becomes `None` because if we do not explicitly return something, Python will insert `return None`.

Example on a function without return value

Let us make a table of $L(x; n)$ versus the exact $\ln(1 + x)$:

```
def table(x):
    print '\nx=%g, ln(1+x)=%g' % (x, log(1+x))
    for n in [1, 2, 10, 100, 500]:
        value, next, error = L2(x, n)
        print 'n=%-4d %-10g  (next term: %8.2e  '\
              'error: %8.2e)' % (n, value, next, error)
```

No need to return anything here - the purpose is to print.

```
x=10, ln(1+x)=2.3979
n=1     0.909091     (next term: 4.13e-01  error: 1.49e+00)
n=2     1.32231      (next term: 2.50e-01  error: 1.08e+00)
n=10    2.17907      (next term: 3.19e-02  error: 2.19e-01)
n=100   2.39789      (next term: 6.53e-07  error: 6.59e-06)
n=500   2.3979       (next term: 3.65e-24  error: 6.22e-15)
```

Keyword arguments are useful to simplify function calls and help document the arguments

Functions can have arguments of the form `name=value`, called *keyword arguments*:

```
>>> def somefunc(arg1, arg2, kwarg1=True, kwarg2=0):
>>>     print arg1, arg2, kwarg1, kwarg2

>>> somefunc('Hello', [1,2])   # drop kwarg1 and kwarg2
Hello [1, 2] True 0            # default values are used

>>> somefunc('Hello', [1,2], kwarg1='Hi')
Hello [1, 2] Hi 0              # kwarg2 has default value

>>> somefunc('Hello', [1,2], kwarg2='Hi')
Hello [1, 2] True Hi           # kwarg1 has default value

>>> somefunc('Hello', [1,2], kwarg2='Hi', kwarg1=6)
Hello [1, 2] 6 Hi              # specify all args
```

If we use `name=value` for *all* arguments *in the call*, their sequence can in fact be arbitrary:

```
>>> somefunc(kwarg2='Hello', arg1='Hi', kwarg1=6, arg2=[2])
Hi [2] 6 Hello
```

Example: Mathematical function of one variable, but with additional parameteres

Consider a function of t, with parameters A, a, and ω:

$$f(t; A, a, \omega) = Ae^{-at}\sin(\omega t)$$

We can implement f in a Python function with t as positional argument and A, a, and ω as keyword arguments:

```
from math import pi, exp, sin

def f(t, A=1, a=1, omega=2*pi):
    return A*exp(-a*t)*sin(omega*t)

v1 = f(0.2)
v2 = f(0.2, omega=1)
v2 = f(0.2, 1, 3)   # same as f(0.2, A=1, a=3)
v3 = f(0.2, omega=1, A=2.5)
v4 = f(A=5, a=0.1, omega=1, t=1.3)
v5 = f(t=0.2, A=9)
v6 = f(t=0.2, 9)    # illegal: keyword arg before positional
```

Doc strings

Python convention: document the purpose of a function, its arguments, and its return values in a *doc string* - a (triple-quoted) string written right after the function header.

```
def C2F(C):
    """Convert Celsius degrees (C) to Fahrenheit."""
    return (9.0/5)*C + 32

def line(x0, y0, x1, y1):
    """
    Compute the coefficients a and b in the mathematical
    expression for a straight line y = a*x + b that goes
    through two points (x0, y0) and (x1, y1).

    x0, y0: a point on the line (floats).
    x1, y1: another point on the line (floats).
    return: a, b (floats) for the line (y=a*x+b).
    """
    a = (y1 - y0)/(x1 - x0)
    b = y0 - a*x0
    return a, b
```

Convention for input and output data in functions

- A function can have three types of input and output data:
  - input data specified through positional/keyword arguments
  - input/output data given as positional/keyword arguments that will be modified and returned
  - output data created inside the function
- *All output data are returned, all input data are arguments*

```
def somefunc(i1, i2, i3, io4, io5, i6=value1, io7=value2):
    # modify io4, io5, io7; compute o1, o2, o3
    return o1, o2, o3, io4, io5, io7
```

The function arguments are

- pure input: `i1, i2, i3, i6`
- input and output: `io4, io5, io7`

The main program

The *main program* is the set of statements outside functions.

```
from math import *           # in main

def f(x):                    # in main
    e = exp(-0.1*x)
    s = sin(6*pi*x)
    return e*s

x = 2                        # in main
y = f(x)                     # in main
print 'f(%g)=%g' % (x, y)    # in main
```

The execution starts with the first statement in the main program and proceeds line by line, top to bottom.
`def` statements define a function, but the statements inside the function are not executed before the function is called.

Python functions as arguments to Python functions

- Programs doing calculus frequently need to have functions as arguments in other functions
- For example:
  - numerical integration: $\int_a^b f(x)dx$
  - numerical differentiation: $f'(x)$
  - numerical root finding: $f(x) = 0$
- All the three functions need f, as a Python function

Example: numerical computation of $f''(x)$ by

$$f''(x) \approx \frac{f(x-h) - 2f(x) + f(x+h)}{h^2}$$

```
def diff2(f, x, h=1E-6):
    r = (f(x-h) - 2*f(x) + f(x+h))/float(h*h)
    return r
```

No difficulty with `f` being a function (more complicated in Matlab, C, C++, Fortran, Java, ...).

Application of the `diff2` function

Code:

```
def g(t):
    return t**(-6)

# make table of g''(t) for 14 h values:
for k in range(1,15):
    h = 10**(-k)
    print 'h=%.0e: %.5f' % (h, diff2(g, 1, h))
```

Output ($g''(1) = 42$):

```
h=1e-01: 44.61504
h=1e-02: 42.02521
h=1e-03: 42.00025
h=1e-04: 42.00000
h=1e-05: 41.99999
h=1e-06: 42.00074
h=1e-07: 41.94423
h=1e-08: 47.73959
h=1e-09: -666.13381
h=1e-10: 0.00000
h=1e-11: 0.00000
h=1e-12: -666133814.77509
h=1e-13: 66613381477.50939
h=1e-14: 0.00000
```

Round-off errors caused nonsense values in the table

- For $h < 10^{-8}$ the results are totally wrong!
- We would expect better approximations as h gets smaller
- Problem 1: for small h we subtract numbers of approx equal size and this gives rise to round-off errors
- Problem 2: for small h the round-off errors are multiplied by a big number
- Remedy: use float variables with more digits
- Python has a (slow) float variable with arbitrary number of digits
- Using 25 digits gives accurate results for $h \leq 10^{-13}$
- Is this really a problem? Quite seldom - other uncertainties in input data to a mathematical computation makes it usual to have (e.g.) $10^{-2} \leq h \leq 10^{-6}$

Lambda functions for compact inline function definitions

```
def f(x):
    return x**2 - 1
```

The *lambda* construction can define this function in one line:

```
f = lambda x: x**2 - 1
```

In general,

```
somefunct = lambda a1, a2, ...: some_expression
```

is equivalent to

```
def somefunc(a1, a2, ...):
    return some_expression
```

Lambda functions can be used directly as arguments in function calls:

```
value = someotherfunc(lambda x, y, z: x+y+3*z, 4)
```

Example on using a lambda function to save typing

Old code:

```
def g(t):
    return t**(-6)

print diff2(g)
```

New, more compact code with lambda:

```
print diff2(lambda t: t**(-6))
```

If tests for branching the flow of statements

Sometimes we want to peform different actions depending on a condition. Example:

$$f(x) = \begin{cases} \sin x, & 0 \leq x \leq \pi \\ 0, & \text{otherwise} \end{cases}$$

A Python implementation of f needs to test on the value of x and branch into two computations:

```
def f(x):
    if 0 <= x <= pi:
        return sin(x)
    else:
        return 0
```

In general (the `else` block can be skipped):

```
if condition:
    <block of statements, executed if condition is True>
else:
    <block of statements, executed if condition is False>
```

If tests with multiple branches

We can test for multiple (here 3) conditions:

```
if condition1:
    <block of statements>
elif condition2:
    <block of statements>
elif condition3:
    <block of statements>
else:
    <block of statements>
<next statement>
```

Example on multiple branching

Here is a piecewisely defined function:

$$N(x) = \begin{cases} 0, & x < 0 \\ x, & 0 \le x < 1 \\ 2 - x, & 1 \le x < 2 \\ 0, & x \ge 2 \end{cases}$$

```
def N(x):
    if x < 0:
        return 0
    elif 0 <= x < 1:
        return x
    elif 1 <= x < 2:
        return 2 - x
    elif x >= 2:
        return 0
```

Inline if tests for shorter code

A common construction is

```
if condition:
    variable = value1
else:
    variable = value2
```

This test can be placed on one line as an expression:

```
variable = (value1 if condition else value2)
```

Example:

```
def f(x):
    return (sin(x) if 0 <= x <= 2*pi else 0)
```

Test functions

Good habit:

To verify the implementation of a function, write a separate function according to some rules.
Example:

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

def test_double():
    x = 4
    exact_result = 8
    r = double(x)
    assert r == exact_result, 'got %s, should have %s' % \
        (r, exact_result)
```

Rules for test functions:

- name begins with `test_`
- no arguments
- must have an `assert condition` statement, where `condition` is `True` if the test passed and `False` otherwise (can have optional message, which is printed if test failed)

Why write test functions according to these rules?

- Easy to recognize where functions are verified
- Test frameworks, like nose and pytest, can automatically run *all* your test functions (in a folder tree) and report if any bugs have sneaked in

```
Terminal> nosetests -s .
Terminal> pytest -s .
```

A test function as `test_double()` is often referred to as a *unit test* since it tests a small unit (function) of a program. When all unit tests work, the whole program is supposed to work.

Summary of if tests and functions

If tests:

```
if x < 0:
    value = -1
elif x >= 0 and x <= 1:
    value = x
else:
    value = 1
```

User-defined functions:

```
def quadratic_polynomial(x, a, b, c)
    value = a*x*x + b*x + c
    derivative = 2*a*x + b
    return value, derivative

# function call:
x = 1
p, dp = quadratic_polynomial(x, 2, 0.5, 1)
p, dp = quadratic_polynomial(x=x, a=-4, b=0.5, c=0)
```

Positional arguments must appear before keyword arguments:

```
def f(x, A=1, a=1, w=pi):
    return A*exp(-a*x)*sin(w*x)
```

A summarizing example for Chapter 3; problem

An integral

$$\int_a^b f(x)dx$$

can be approximated by *Simpson's rule*:

$$\int_a^b f(x)dx \approx \frac{b-a}{3n}\left(f(a) + f(b) + 4\sum_{i=1}^{n/2} f(a + (2i-1)h) + 2\sum_{i=1}^{n/2-1} f(a + 2ih)\right)$$

Problem: make a function `Simpson(f, a, b, n=500)` for computing an integral of `f(x)` by Simpson's rule. Call `Simpson(...)` for $\frac{3}{2}\int_0^\pi \sin^3 x dx$ (exact value: 2) for $n = 2, 6, 12, 100, 500$.

The program: function for computing the formula

```
def Simpson(f, a, b, n=500):
    """
    Return the approximation of the integral of f
    from a to b using Simpson's rule with n intervals.
    """

    h = (b - a)/float(n)

    sum1 = 0
    for i in range(1, n/2 + 1):
        sum1 += f(a + (2*i-1)*h)

    sum2 = 0
    for i in range(1, n/2):
        sum2 += f(a + 2*i*h)

    integral = (b-a)/(3*n)*(f(a) + f(b) + 4*sum1 + 2*sum2)
    return integral
```

The program: function, now with test for possible errors

```
def Simpson(f, a, b, n=500):

    if a > b:
        print 'Error: a=%g > b=%g' % (a, b)
        return None

    # Check that n is even
    if n % 2 != 0:
        print 'Error: n=%d is not an even integer!' % n
        n = n+1  # make n even

    # as before...
    ...
    return integral
```

The program: application (and main program)

```
def h(x):
    return (3./2)*sin(x)**3

from math import sin, pi

def application():
    print 'Integral of 1.5*sin^3 from 0 to pi:'
    for n in 2, 6, 12, 100, 500:
        approx = Simpson(h, 0, pi, n)
        print 'n=%3d, approx=%18.15f, error=%9.2E' % \
              (n, approx, 2-approx)

application()
```

The program: verification (with test function)

Property of Simpson's rule: 2nd degree polynomials are integrated exactly!

```
def test_Simpson():      # rule: no arguments
    """Check that 2nd-degree polynomials are integrated exactly."""
    a = 1.5
    b = 2.0
    n = 8
    g = lambda x: 3*x**2 - 7*x + 2.5       # test integrand
    G = lambda x: x**3 - 3.5*x**2 + 2.5*x  # integral of g
    exact = G(b) - G(a)
    approx = Simpson(g, a, b, n)
    success = abs(exact - approx) < 1E-14  # tolerance for floats
    msg = 'exact=%g, approx=%g' % (exact, approx)
    assert success, msg   # assert boolean success condition
```

Can either call `test_Simpson()` or run nose or pytest:

```
Terminal> nosetests -s Simpson.py
Terminal> pytest -s Simpson.py
...
Ran 1 test in 0.005s

OK
```