

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: $y(t) = v_0 t - \frac{1}{2} g t^2$. 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

```
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:

```
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 $y(t, v_0)$ function took two arguments. Could implement $y(t)$ as a function of t only:

```
>>> 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: v_0 must be defined in the calling program before we call `yfunc`

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

Note:

- v_0 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 $y'(t) = v_0 - gt$:

```
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:

```
>>> 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 $L(x; n)$:

```
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 ($\ln(1+x) - L(x; n)$):

```
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

```
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 '\n'  
              '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 parameters

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,

```
somefunc = 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 perform 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:

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

```
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