

Ch.3: Functions and branching

Hans Petter Langtangen^{1,2}

Simula Research Laboratory¹
University of Oslo, Dept. of Informatics²

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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)  
integers = 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!

Functions are one of the most important tools in programming

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

Python function for implementing a mathematical function

The mathematical function

$$F(C) = \frac{9}{5}C + 32$$

can be implemented in Python as follows:

```
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

```
def F(C):  
    return (9.0/5)*C + 32  
  
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 [0, 20, 40]] # multiple calls
```

(Visualize execution)

Note:

The call `F(C)` produces (returns) a float object, which means that `F(C)` is replaced by this float object. We can therefore make the call `F(C)` everywhere a float can be used.

Functions can have as many arguments as you like

Make a Python function of the mathematical function

$$y(t) = v_0t - \frac{1}{2}gt^2$$

```
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)
```

(Visualize execution)

Function arguments become local variables

```
def yfunc(t, v0):  
    g = 9.81  
    return v0*t - 0.5*g*t**2  
  
v0 = 5  
t = 0.6  
y = yfunc(t, 3)
```

(Visualize execution)

Local vs global variables

When calling `yfunc(t, 3)`, all these statements are in fact executed:

```
t = 0.6 # arguments get values as in standard assignments  
v0 = 3  
g = 9.81  
return v0*t - 0.5*g*t**2
```

Inside `yfunc`, `t`, `v0`, and `g` are *local variables*, not visible outside `yfunc` and destroyed after return.

Outside `yfunc` (in the main program), `t`, `v0`, and `y` are *global variables*, visible everywhere.

Functions may access global variables

The `yfunc(t, v0)` 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  
...  
>>> t = 0.6  
>>> yfunc(t)  
...  
NameError: global name 'v0' is not defined
```

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

```
>>> v0 = 5  
>>> yfunc(0.6)  
1.2942
```

Note: `v0` and `t` (in the main program) are global variables, while the `t` in `yfunc` is a local variable.

Local variables hide global variables of the same name

Test this:

```
def yfunc(t):  
    print '1. local t inside yfunc:', t  
    g = 9.81  
    t = 0.1  
    print '2. local t inside yfunc:', t  
    return v0*t - 0.5*g*t**2  
  
t = 0.6  
v0 = 2  
print yfunc(t)  
print '1. global t:', t  
print yfunc(0.3)  
print '2. global t:', t
```

(Visualize execution)

Question

What gets printed?

Global variables can be changed if declared global

```
def yfunc(t):  
    g = 9.81  
    global v0 # now v0 can be changed inside this function  
    v0 = 9  
    return v0*t - 0.5*g*t**2  
  
v0 = 2 # global variable  
print '1. v0:', v0  
print yfunc(0.8)  
print '2. v0:', v0
```

(Visualize execution)

What gets printed?

```
1. v0: 2  
4.0608  
2. v0: 9
```

What happens if we comment out `global v0`?

```
1. v0: 2  
4.0608  
2. v0: 2
```

`v0` in `yfunc` becomes a local variable (i.e., we have two `v0`)

Functions can return multiple values

Say we want to compute `y(t)` and `y'(t) = v0 - 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) # same syntax as x, y = (obj1, obj2)
```

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 $x \geq 1$.

Corresponding 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: 1) the first neglected term in the sum and 2) 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

Make a table of $L(x; n)$ vs. $\ln(1+x)$:

```
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=1.0, 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
```

Examples on calling functions with 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
```

How to implement a mathematical function of one variable, but with additional parameters?

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

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

Possible implementation

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

Doc strings are used to document the usage of a function

Important 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 = ax + 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=ax+b).
    """
    a = (y1 - y0)/(x1 - x0)
    b = y0 - ax0
    return a, b
```

Python convention: input is function arguments, output is returned

- 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, i4, i5, i6=value1, i7=value2):
    # modify i04, i05, i07; compute o1, o2, o3
    return o1, o2, o3, i04, i05, i07
```

The function arguments are

- pure input: i1, i2, i3, i6
- input and output: i04, i05, i07

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(0*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, e.g.,
 - numerical integration: $\int_a^b f(x) dx$
 - numerical differentiation: $f'(x)$
 - numerical root finding: $f(x) = 0$
- All three cases need f as a Python function $f(x)$

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

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

```
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 (read the output!)

Code:

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

# make table of g''(t) for 13 h values:
for k in range(1,14):
    h = 10**(-k)
    print 'h=%0a: %.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
```

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 (decimal.Decimal) 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

Verbose standard code:

```
def g(t):  
    return t**(-6)  
  
dgd_t = diff2(g, 2)  
print dgd_t
```

More compact code with lambda:

```
dgd_t = diff2(lambda t: t**(-6), 2)  
print dgd_t
```

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:

```
from math import sin, pi  
  
def f(x):  
    if 0 <= x <= pi:  
        return sin(x)  
    else:  
        return 0  
  
print f(0.5)  
print f(5*pi)
```

(Visualize execution)

The general form of if tests

if-else (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>
```

Multiple if-else

```
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

A piecewisely defined function

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

Python implementation with multiple if-else-branching

```
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

Common construction:

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

More compact syntax with one-line if-else:

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

Example:

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

We shall write special *test functions* to verify functions

```
def double(x):
    # some function
    return 2*x

def test_double():
    # associated test function
    """Call double(x) to check that it works."""
    x = 4
    # some chosen x value
    expected = 8
    computed = double(x)
    success = computed == expected # boolean value: test passed?
    msg = 'computed %s, expected %s' % (computed, expected)
    assert success, msg
```

Rules for test functions:

- name begins with test_
- no arguments
- must have an assert success statement, where success is True if the test passed and False otherwise (assert success, msg prints msg on failure)

The optional msg parameter writes a message if the test fails.

Test functions with many tests

```
def double(x):
    # some function
    return 2*x

def test_double():
    # associated test function
    tol = 1E-14 # tolerance for float comparison
    x_values = [3, 7, -2, 0, 4.5, 'hello']
    expected_values = [6, 14, -4, 0, 9, 'hellohello']
    for x, expected in zip(x_values, expected_values):
        computed = double(x)
        msg = '%s != %s' % (computed, expected)
        assert abs(expected - computed) < tol, msg
```

A test function *will run silently* if all tests pass. If one test above fails, assert will raise an AssertionError.

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
- This is a very well established standard

```
Terminal> py.test -s .
Terminal> nosetests -s .
```

We recommend `py.test` - it has superior output.

Unit tests

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.

Comments on test functions

- Many find test functions to be a difficult topic
- The idea *is* simple: make problem where you know the answer, call the function, compare with the known answer
- Just write some test functions and it will be easy
- The fact that a successful test function runs silently is annoying - can (during development) be convenient to insert some print statements so you realize that the statements are run

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 quadratic functions 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
```

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

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