

Ch.3: Functions and branching

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Today's agenda

- A brief recap of the last lecture
- A small quiz
- Live-programming of exercises 3.20, 3.23, 3.28
- More about functions + branching

Short recap of functions

Defining a function in Python

```
def f(x):  
    return 2 * x**2 + x
```

Using a function in Python

```
x = -0.6  
print(f(x))          # 0.12  
print(f(x**2))      # 0.6192
```

Python functions can have local variables

```
a = 0.5              # Global variable  
  
def g(x):  
    a = 0.6323      # Local variable  
    b = a*x + 1  
    return b  
  
print(a)             # a is 0.5  
print(g(0))  
print(a)             # a is still 0.5
```

Local variables can hide global variables

If a local variable and a global variable have the same name, only the local variable is visible inside the function.

Example:

```
def g(t):  
    alpha = 1.0  
    beta = 2.0  
    return alpha + beta*t  
  
print(g(1))           # Prints out '3.0'  
alpha = 10.0  
print(g(1))           # Still prints out '3.0'
```

In this example, the value `alpha = 10.0` is never actually used.

What is the purpose of hiding global variables?

- It can be very useful to access global variables inside a function, for example to access constants defined outside the function.
- Still, the rule is that when a name collision occurs, the local variable "wins" and the global variable becomes invisible
- Why? Because otherwise it would be impossible to know how a function would behave when used in new contexts (with new global variables).

Changing global variables in a function

Suppose we wanted to change the value of a global variable from inside a function. Not as easy as it seems:

```
x = 10
def f(y):
    x = 5    # We try to change the global variable
    return x + y

print(x)    # Prints out '10'
print(f(0)) # Prints out '5'
print(x)    # Prints out '10' (so the global variable x is still 10!)
```

Attempting to change a global variable inside a function fails in this case, because we inadvertently define a *local* variable *x* when we write *x=5*.

Changing global variables in a function (2)

- If we really want to change a global variable inside a function, we have to declare the variable as *global*.
- However, you should *only* do this if you really have to.

Example:

```
x = 10
def f(y):
    global x           # This says: don't create a local variable x
    x = 5             # This time we do change the global variable
    return x + y

print(x)             # Prints out '10'
print(f(0))         # Prints out '5'
print(x)             # Prints out '5' (so the global variable x is changed)
```

Example: Compute a function defined as a sum

This function approximates $\ln(1+x)$ for $x \geq 1$:

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

Corresponding Python function:

```
def L(x,n):  
    s = 0  
    for i in range(1, n+1):  
        s += (1.0/i)*(x/(1.0+x))**i  
    return s
```

Example of use:

```
import math  
x = 5.0  
print (L(x, 10), L(x, 100), math.log(1+x))
```


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

Suppose we want to return more information about the approximation:

- The first neglected term in the sum
- The error $(\ln(1 + x) - L(x; n))$

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

typical call:

```
x = 1.2; n = 100
```

```
value, approximate_error, exact_error = L2(x, n)
```

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

Functions can have arguments of the form `name=value`, and these are called *keyword arguments*.

Example:

```
def printAll(x, y, z=1, w=2.5):  
    print(x, y, z, w)
```

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
```

Quiz 1

If `a = ['A', ['B', ['B', 'C']]]` then which of the expressions below are equal to B?

- `a[0]`
- `a[1][1]`
- `a[2][0]`
- `a[1][-2]`
- `a[-1][0]`
- `a[1][1][0]`
- `a[a.index('B')]`
- `a[len(a)-1][len(a)-1][0]`

Quiz 2

Creating lists

- Create the list `a = ['A', 'A', ..., 'A']` of length 5000
- Create the list `b = ['A0', 'A1', ..., 'A4999']`

Equal or not?

Suppose `a = [0, 2, 4, 6, 8, 10]`. Which of the expressions below are equal to `True`?

- `a[0] == a[-6]`
- `a[1] == a[-5]`
- `a[1:4] == [2, 4, 6, 8]`
- `a[1:4] == [a[i] for i in range(1,4)]`
- `a is a`
- `a[:] is a`

Quiz 3

Suppose the following statements are performed:

```
a = [0, 1, 2, 3, 4]
b = a
b[0] = 50
print(a[0], b[0])
```

What is printed out here?

Quiz 4

Suppose the following statements are performed:

```
a = [0, 1, 2, 3, 4]
b = a[:]
b[0] = 50
print(a[0], b[0])
```

What is printed out here?

Suppose we have defined a function

```
def h(x, y, z=0):  
    import math  
    res = x * math.sin(y) + z  
    return res
```

Which of these function calls are allowed?

- $r = h(0)$
- $r = h(0, 1)$
- $r = h(0, 1, 2)$
- $r = h(x=0, 1, 2)$
- $r = h(0, y=1)$
- $r = h(0, 1, z=3)$
- $r = h(0, 0, x=0)$
- $r = h(z=0, x=1)$
- $r = h(z=0, x=1, y=2)$

What is printed out here:

```
def myfunc(k):  
    x = k * 2  
    print('x = %g' % x)
```

```
x = 5  
print('x = %g' % x)  
myfunc(5)  
print('x = %g' % x)
```

Exercise 3.20

Write functions

Three functions `hw1`, `hw2`, and `hw3` work as follows:

```
>>> print(hw1())
>>> Hello, World
>>>
>>> hw2()
>>> Hello, World
>>>
>>> print(hw3('Hello, ', 'World'))
>>> Hello, World
>>>
>>> print(hw3('Python ', 'function'))
>>> Python function
```

Write the three functions.

Filename: `hw_func`.

Exercise 3.23

Wrap a formula in a function

Implement the formula (1.9) from Exercise 1.12 in a Python function with three arguments: `egg(M, To=20, Ty=70)`.

$$t = \frac{M^{2/3} c \rho^{1/3}}{K \pi^2 (4\pi/3)^{2/3}} \ln \left[0.76 \frac{T_0 - T_w}{T_y - T_w} \right].$$

The parameters ρ , K , c , and T_w can be set as local (constant) variables inside the function. Let t be returned from the function. Compute t for these conditions:

- Soft ($T_y < 70$) and hard boiled ($T_y > 70$)
- Small ($M = 47\text{g}$) and large ($M = 67\text{g}$) egg
- Fridge ($T_0 = 4\text{C}$) and hot room ($T_0 = 25\text{C}$).

Filename: `egg_func`.

Exercise 3.28

Find the max and min elements in a list

Given a list `a`, the `max` function in Python's standard library computes the largest element in `a`: `max(a)`. Similarly, `min(a)` returns the smallest element in `a`.

Write your own `max` and `min` functions.

Hint: Initialize a variable `max_elem` by the first element in the list, then visit all the remaining elements (`a[1:]`), compare each element to `max_elem`, and if greater, set `max_elem` equal to that element. Use a similar technique to compute the minimum element.

Filename: `maxmin_list`.

More about functions: an example

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

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

Possible implementation in Python:

```
from math import pi, exp, sin

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

Observe that t is a positional argument, while A , a , and ω are keyword arguments. That gives us large freedom when calling the function:

```
v1 = f(0.2) # Only give t
v2 = f(0.2, omega=1) # Change default value of omega
v3 = f(0.2, omega=1, A=2.5) # Change default value of omega and A
v4 = f(A=5, a=0.1, omega=1, t=1.3) # Change all three parameters
v5 = f(0.2, 1, 2.5) # Change default value of A and a
```

Even functions can be used as arguments in functions

In Python, functions are allowed to take functions as arguments. Thus we can "pass on" a function to another function.

Example: If we know how to compute $f(x)$ then we can use the following approximation to find numerically the 2nd derivative of $f(x)$ in a given point:

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

Python implementation:

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

Here, the first argument to `diff2(.)` is a function.

The function we just defined had one keyword argument $h=1E-6$. Is there any good reason to choose $h = 0.000001$ rather than a smaller or larger value?

- Mathematically, we expect the approximation to improve when h gets smaller.
- However, when we solve problems numerically we also need to take into account rounding errors.
- Some numerical problems are more sensitive to rounding errors than others, so in practice we may have to do a bit of trial and error.

The effect of changing the value of h

To study the effect of changing h we write a small program:

```
def g(t):  
    return t**(-6)  
  
# Compute  $g''(t)$  for smaller and smaller values of  $h$ :  
for k in range(1,14):  
    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
```


Rounding errors dominate for small h-values

For $h < 10^{-8}$ the results are totally wrong!

- **Problem 1:** for small h we subtract numbers of roughly equal size and this gives rise to rounding error.
- **Problem 2:** for small h the rounding error is divided by a very small number (h^2), which amplifies the error.

Possible solution: 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 $h \leq 10^{-13}$

However, higher accuracy is rarely needed in practice.

Functions vs. main program

The *main program* is the part of the program that is not inside any functions. In general:

- Execution starts with the first statement in the main program and proceeds line by line, top to bottom.
- Functions are only executed when they are called

Note: functions can be called from the main program *or* from a function. During program execution, this can sometimes result in long "chains" of function calls.

Anonymous functions (lambda functions)

Sometimes a function just involves the calculation of an expression. In that case, we can use the *lambda construction* to define it.

Example: the function

```
def f(x,y):  
    return x**2 - y**2
```

can be defined in just one line with the lambda construction:

```
f = lambda x, y: x**2 - y**2
```

Lambda functions can be used directly as arguments:

```
z = g(lambda x, y: x**2 - y**2, 4)
```

Can you guess why lambda functions are also called anonymous functions?

Documenting functions is important

To add a brief description (*doc string*) to a function, place it right after the function header and inside triple quotes.

Examples:

```
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 expression for a  
    straight line  $y = a*x + b$  through two specified points.  
  
    x0, y0: the first point (floats).  
    x1, y1: the second point (floats).  
    return: a, b (floats) for the line ( $y=a*x+b$ ).  
    """  
    a = (y1 - y0)/(x1 - x0)  
    b = y0 - a*x0  
    return a, b
```

An if-test allows the program to take different actions depending on what the current state of the program is. An if-test thus branches (splits) the flow of actions.

Example: consider the function

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

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
```

General form of an if-test

Type 1 (if)

```
if condition:  
    <block of statements, executed when condition==True>
```

Type 2 (if-else)

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

Type 3 (if-elif-else)

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

Example 1

A piecewise 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 if-elif-else:

```
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
```

Example 2

The following function counts how many times `s` occurs in `a`:

```
def count(s, a):
    cnt = 0
    for e in a:
        if e == s:
            cnt += 1
    return cnt
```

Example of use:

```
>>> count(5.3, [2.2, 6.6, 2.5, 5.3, 8.9, 5.3])
>>> 2
>>>
>>> count('Anna', ['Ola', 'Karianne', 'Anna', 'Jens'])
>>> 1
>>>
>>> count([1,2], [1, 5, [1,2], [1,2], 3])
>>> 2
```


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)
```

A very special form of if-test: assert

Sometimes in a program you want to stop program execution and give an error message if a condition is not true. For this purpose, we can use the assert statement. General form:

```
assert condition, message
```

Example:

```
>>> x = 5
>>> assert x > 0, "x should be positive" # Nothing happens
>>> x = -5
>>> assert x > 0, "x should be positive" # Generates error message
Traceback (most recent call last):

  File "<ipython-input-30-c680011d20e2>", line 1, in <module>
    assert x > 0, "x should be positive"

AssertionError: x should be positive
```

Writing test functions

Suppose we have written a new function with some return values. To convince ourselves it works properly, we should try it for some input values and see if the result matches what we expect.

Note: the strategy above only works if we actually know what the answer *should* be. Often we know this for some input values.

Test strategy

- Write the new function.
- Write a *test function* that calls the new function with input values chosen so we know what the output should be.
- If the output from the new function differs from the expected output, we stop execution and print an error message.

Example

```
def sum3(a):          # Find sum of every 3rd element in a
    res = sum([a[i] for i in range(0,len(a),3)])
    return res

def test_sum3():     # Associated test function
    """Call sum3(a) to check that it works."""
    a = [0,1,2,3,4,5] # Some chosen input value
    expected = 3      # What the output should be
    computed = sum3(a)
    success = (computed == expected) # Did the test pass?
    message = 'computed %s, expected %s' % (computed, expected)
    assert success, message
```

Test functions with many tests

```
def sum3(a):          # Find sum of every 3rd element in a
    res = sum([a[i] for i in range(0,len(a),3)])
    return res

def test_sum3():     # Associated test function
    """Call sum3(a) to check that it works."""
    tol = 1E-14
    inputs = [[6], [6,1], [6,1,2], [6,1,2,3]]
    answers = [6, 6, 6, 9]
    for a, expected in zip(inputs, answers):
        computed = sum3(a)
        message = '%s != %s' % (computed, expected)
        assert abs(expected - computed) < tol, message
```

Recall that `zip(a, b)` creates pairs `[a[i],b[i]]`:

```
>>> zip(inputs, answers)
>>> [( [6], 6), ([6, 1], 6), ([6, 1, 2], 6), ([6, 1, 2, 3], 9)]
```

More about test functions

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

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.

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*:

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

where n is an even integer.

Problem: make a function `Simpson(f, a, b, n=500)` for computing an integral of $f(x)$ by Simpson's rule.

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