Functions and branching

3

This chapter introduces two fundamental and extremely useful concepts in programming: user-defined functions and branching of program flow, the latter often referred to as `if` tests. The programs associated with the chapter are found in the folder `src/funcif`[1].

3.1 Functions

In a computer language like Python, the term *function* means more than just a mathematical function. A function is a collection of statements that you can execute wherever and whenever you want in the program. You may send variables to the function to influence what is getting computed by statements in the function, and the function may return new objects back to you.

In particular, functions help avoid duplicating code snippets by putting all similar snippets in a common place. This strategy saves typing and makes it easier to change the program later. Functions are also often used to just split a long program into smaller, more manageable pieces, so the program and your own thinking about it become clearer. Python comes with lots of pre-defined functions (`math.sqrt`, `range`, and `len` are examples we have met so far). This section explains how you can define your own functions.

3.1.1 Mathematical functions as Python functions

Let us start with making a Python function that evaluates a mathematical function, more precisely the function $F(C)$ for converting Celsius degrees C to the corresponding Fahrenheit degrees F:

[1] `http://tinyurl.com/pwyasaa/funcif`

H.P. Langtangen, *A Primer on Scientific Programming with Python*,
Texts in Computational Science and Engineering 6,
DOI 10.1007/978-3-642-54959-5_3, © Springer-Verlag Berlin Heidelberg 2014

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

The corresponding Python function must take C as argument and return the value $F(C)$. The code for this looks like

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

All Python functions begin with `def`, followed by the function name, and then inside parentheses a comma-separated list of *function arguments*. Here we have only one argument `C`. This argument acts as a standard variable inside the function. The statements to be performed inside the function must be indented. At the end of a function it is common to *return* a value, that is, send a value "out of the function". This value is normally associated with the name of the function, as in the present case where the returned value is the result of the mathematical function $F(C)$.

The `def` line with the function name and arguments is often referred to as the *function header*, while the indented statements constitute the *function body*.

To use a function, we must *call* (or *invoke*) it. Because the function returns a value, we need to store this value in a variable or make use of it in other ways. Here are some calls to `F`:

```
temp1 = F(15.5)
a = 10
temp2 = F(a)
print F(a+1)
sum_temp = F(10) + F(20)
```

The returned object from `F(C)` is in our case a `float` object. The call `F(C)` can therefore be placed anywhere in a code where a `float` object would be valid. The `print` statement above is one example.

As another example, say we have a list `Cdegrees` of Celsius degrees and we want to compute a list of the corresponding Fahrenheit degrees using the `F` function above in a list comprehension:

```
Fdegrees = [F(C) for C in Cdegrees]
```

Yet another example may involve a slight variation of our `F(C)` function, where a formatted string instead of a real number is returned:

```
>>> def F2(C):
...     F_value = (9.0/5)*C + 32
...     return '%.1f degrees Celsius corresponds to '\
...            '%.1f degrees Fahrenheit' % (C, F_value)
...
>>> s1 = F2(21)
>>> s1
'21.0 degrees Celsius corresponds to 69.8 degrees Fahrenheit'
```

The assignment to `F_value` demonstrates that we can create variables inside a function as needed.

3.1.2 Understanding the program flow

A programmer must have a deep understanding of the sequence of statements that are executed in the program and be able to simulate by hand what happens with a program in the computer. To help build this understanding, a debugger (see Section F.1) or the Online Python Tutor[2] are excellent tools. A debugger can be used for all sorts of programs, large and small, while the Online Python Tutor is primarily an educational tool for small programs. We shall demonstrate it here.

Below is a program `c2f.py` having a function and a `for` loop, with the purpose of printing out a table for conversion of Celsius to Fahrenheit degrees:

```
def F(C):
    F = 9./5*C + 32
    return F

dC = 10
C = -30
while C <= 50:
    print '%5.1f %.51f' % (C, F(C))
    C += dC
```

We shall now ask the Online Python Tutor to visually explain how the program is executed. Go to `http://www.pythontutor.com/visualize.html`, erase the code there and write or paste the `c2f.py` file into the editor area. Click *Visualize Execution*. Press the forward button to advance one statement at a time and observe the evolution of variables to the right in the window. This demo illustrates how the program jumps around in the loop and up to the `F(C)` function and back again. Figure 3.1 gives a snapshot of the status of variables, terminal output, and what the current and next statements are.

Tip: How does a program actually work?

Every time you are a bit uncertain how the flow of statements progresses in a program with loops and/or functions, go to `http://www.pythontutor.com/visualize.html`, paste in your program and see exactly what happens.

[2] `http://www.pythontutor.com/`

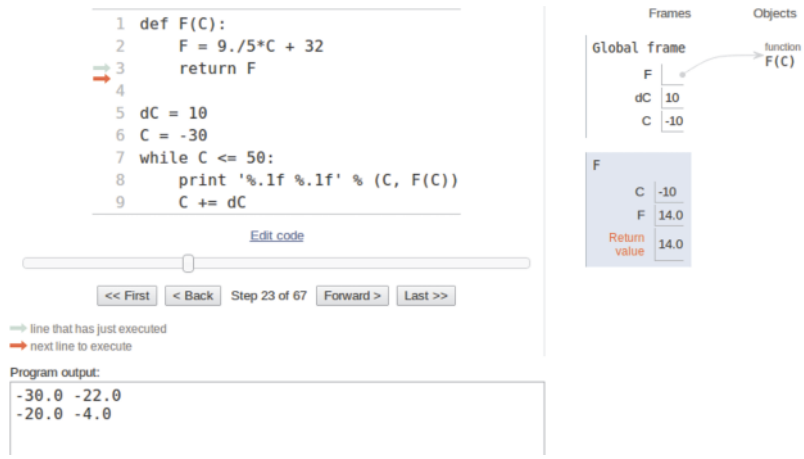


Fig. 3.1 Screen shot of the Online Python Tutor and stepwise execution of the `c2f.py` program.

3.1.3 Local and global variables

Local variables are invisible outside functions. Let us reconsider the `F2(C)` function from Section 3.1.1. The variable `F_value` is a *local* variable in the function, and a local variable does not exist outside the function, i.e., in the main program. We can easily demonstrate this fact by continuing the previous interactive session:

```
>>> c1 = 37.5
>>> s2 = F2(c1)
>>> F_value
...
NameError: name 'F_value' is not defined
```

This error message demonstrates that the surrounding program outside the function is not aware of `F_value`. Also the argument to the function, `C`, is a local variable that we cannot access outside the function:

```
>>> C
...
NameError: name 'C' is not defined
```

On the contrary, the variables defined outside of the function, like `s1`, `s2`, and `c1` in the above session, are *global* variables. These can be accessed everywhere in a program, also inside the `F2` function.

Local variables hide global variables. Local variables are created inside a function and destroyed when we leave the function. To learn more about this fact, we may study the following session where we write out `F_value`, `C`, and some global variable `r` inside the function:

```
>>> def F3(C):
...     F_value = (9.0/5)*C + 32
...     print 'Inside F3: C=%s F_value=%s r=%s' % (C, F_value, r)
...     return '%.1f degrees Celsius corresponds to '\
```

```
...             '%.1f degrees Fahrenheit' % (C, F_value)
...
>>> C = 60    # make a global variable C
>>> r = 21    # another global variable
>>> s3 = F3(r)
Inside F3: C=21 F_value=69.8 r=21
>>> s3
'21.0 degrees Celsius corresponds to 69.8 degrees Fahrenheit'
>>> C
60
```

This example illustrates that there are two `C` variables, one global, defined in the main program with the value 60 (an `int` object), and one local, living when the program flow is inside the `F3` function. The value of this latter `C` is given in the call to the `F3` function (an `int` object). Inside the `F3` function the local `C` *hides* the global `C` variable in the sense that when we refer to `C` we access the local variable. (The global `C` can technically be accessed as `globals()['C']`, but one should avoid working with local and global variables with the same names at the same time!)

The Online Python Tutor gives a complete overview of what the local and global variables are at any point of time. For instance, in the example from Section 3.1.2, Figure 3.1 shows the content of the three global variables `F`, `dC`, and `C`, along with the content of the variables that are in play in this call of the `F(C)` function: `C` and `F`.

How Python looks up variables

The more general rule, when you have several variables with the same name, is that Python first tries to look up the variable name among the local variables, then there is a search among global variables, and finally among built-in Python functions.

Example. Here is a complete sample program that aims to illustrate the rule above:

```
print sum  # sum is a built-in Python function
sum = 500  # rebind the name sum to an int
print sum  # sum is a global variable

def myfunc(n):
    sum = n + 1
    print sum  # sum is a local variable
    return sum

sum = myfunc(2) + 1   # new value in global variable sum
print sum
```

In the first line, there are no local variables, so Python searches for a global value with name `sum`, but cannot find any, so the search proceeds with the built-in functions, and among them Python finds a function with name `sum`. The printout of `sum` becomes something like `<built-in function sum>`.

The second line rebinds the global name `sum` to an `int` object. When trying to access `sum` in the next `print` statement, Python searches among the global variables (no local variables so far) and finds one. The printout becomes `500`. The call `myfunc(2)` invokes a function where `sum` is a local variable. Doing a `print sum` in this function makes Python first search among the local variables, and since `sum` is found there, the printout becomes `3` (and not `500`, the value of the global variable `sum`). The value of the local variable `sum` is returned, added to `1`, to form an `int` object with value `4`. This `int` object is then bound to the global variable `sum`. The final `print sum` leads to a search among global variables, and we find one with value `4`.

Changing global variables inside functions. The values of global variables can be accessed inside functions, but the values cannot be changed unless the variable is declared as `global`:

```
a = 20; b = -2.5        # global variables

def f1(x):
    a = 21              # this is a new local variable
    return a*x + b

print a                 # yields 20

def f2(x):
    global a
    a = 21              # the global a is changed
    return a*x + b

f1(3); print a          # 20 is printed
f2(3); print a          # 21 is printed
```

Note that in the `f1` function, `a = 21` creates a local variable `a`. As a programmer you may think you change the global `a`, but it does not happen! *You are strongly encouraged to run the programs in this section in the Online Python Tutor*, which is an excellent tool to explore local versus global variables and thereby get a good understanding of these concepts.

3.1.4 Multiple arguments

The previous `F(C)` and `F2(C)` functions from Section 3.1.1 are functions of one variable, `C`, or as we phrase it in computer science: the functions take one argument (`C`). Functions can have as many arguments as desired; just separate the argument names by commas.

Consider the mathematical function

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

where g is a fixed constant and v_0 is a physical parameter that can vary. Mathematically, y is a function of one variable, t, but the function values

also depends on the value of v_0. That is, to evaluate y, we need values for t *and* v_0. A natural Python implementation is therefore a function with two arguments:

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

Note that the arguments `t` and `v0` are local variables in this function. Examples on valid calls are

```
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)
```

The possibility to write `argument=value` in the call makes it easier to read and understand the call statement. With the `argument=value` syntax for all arguments, the sequence of the arguments does not matter in the call, which here means that we may put `v0` before `t`. When omitting the `argument=` part, the sequence of arguments in the call must perfectly match the sequence of arguments in the function definition. The `argument=value` arguments must appear after all the arguments where only `value` is provided (e.g., `yfunc(t=0.1, 6)` is illegal).

Whether we write `yfunc(0.1, 6)` or `yfunc(v0=6, t=0.1)`, the arguments are initialized as local variables in the function in the same way as when we assign values to variables:

```
    t = 0.1
    v0 = 6
```

These statements are not visible in the code, but a call to a function automatically initializes the arguments in this way.

3.1.5 Function argument of global variable?

Since y mathematically is considered a function of one variable, t, some may argue that the Python version of the function, `yfunc`, should be a function of `t` only. This is easy to reflect in Python:

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

The main difference is that `v0` now becomes a *global* variable, which needs to be initialized outside the function `yfunc` (in the main program) before we attempt to call `yfunc`. The next session demonstrates what happens if we fail to initialize such a global variable:

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

The remedy is to define `v0` as a global variable prior to calling `yfunc`:

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

The rationale for having `yfunc` as a function of `t` only becomes evident in Section 3.1.12.

3.1.6 Beyond mathematical functions

So far our Python functions have typically computed some mathematical function, but the usefulness of Python functions goes far beyond mathematical functions. Any set of statements that we want to repeatedly execute under potentially slightly different circumstances is a candidate for a Python function. Say we want to make a list of numbers starting from some value and stopping at another value, with increments of a given size. With corresponding variables `start=2`, `stop=8`, and `inc=2`, we should produce the numbers 2, 4, 6, and 8. Let us write a function doing the task, together with a couple of statements that demonstrate how we call the function:

```
def makelist(start, stop, inc):
    value = start
    result = []
    while value <= stop:
        result.append(value)
        value = value + inc
    return result

mylist = makelist(0, 100, 0.2)
print mylist  # will print 0, 0.2, 0.4, 0.6, ... 99.8, 100
```

Remark 1. The `makelist` function has three arguments: `start`, `stop`, and `inc`, which become local variables in the function. Also `value` and `result` are local variables. In the surrounding program we define only one variable, `mylist`, and this is then a global variable.

Remark 2. You might think that `range(start, stop, inc)` makes the `makelist` function redundant, but `range` can only generate integers, while `makelist` can generate real numbers too, and more, as demonstrated in Exercise 3.38.

3.1.7 Multiple return values

Python functions may return more than one value. Suppose we are interested in evaluating both $y(t)$ and $y'(t)$:

$$y(t) = v_0 t - \frac{1}{2} g t^2,$$
$$y'(t) = v_0 - gt\,.$$

To return both y and y' we simply separate their corresponding variables by a comma in the `return` statement:

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

Calling this latter `yfunc` function makes a need for two values on the left-hand side of the assignment operator because the function returns two values:

```
position, velocity = yfunc(0.6, 3)
```

Here is an application of the `yfunc` function for producing a nicely formatted table of t, $y(t)$, and $y'(t)$ values:

```
t_values = [0.05*i for i in range(10)]
for t in t_values:
    position, velocity = yfunc(t, v0=5)
    print 't=%-10g position=%-10g velocity=%-10g' % \
          (t, position, velocity)
```

The format `%-10g` prints a real number as compactly as possible (decimal or scientific notation) in a field of width 10 characters. The minus sign (-) after the percentage sign implies that the number is *left-adjusted* in this field, a feature that is important for creating nice-looking columns in the output:

```
t=0         position=0          velocity=5
t=0.05      position=0.237737   velocity=4.5095
t=0.1       position=0.45095    velocity=4.019
t=0.15      position=0.639638   velocity=3.5285
t=0.2       position=0.8038     velocity=3.038
t=0.25      position=0.943437   velocity=2.5475
t=0.3       position=1.05855    velocity=2.057
t=0.35      position=1.14914    velocity=1.5665
t=0.4       position=1.2152     velocity=1.076
t=0.45      position=1.25674    velocity=0.5855
```

When a function returns multiple values, separated by a comma in the `return` statement, a tuple (Section 2.5) is actually returned. We can demonstrate that fact by the following session:

```
>>> 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)   # store in separate variables
```

Note that storing multiple return values in separate variables, as we do in the last line, is actually the same functionality as we use for storing list (or tuple) elements in separate variables, see Section 2.2.1.

3.1.8 Computing sums

Our next example concerns a Python function for calculating the sum

$$L(x;n) = \sum_{i=1}^{n} \frac{1}{i}\left(\frac{x}{1+x}\right)^i. \tag{3.1}$$

To compute a sum in a program, we use a loop and add terms to an accumulation variable inside the loop. Section 2.1.4 explains the idea. However, summation expressions with an integer counter, such as i in (3.1), are normally implemented by a `for` loop over the i counter and not a `while` loop as in Section 2.1.4. For example, the implementation of $\sum_{i=1}^{n} i^2$ is typically implemented as

```
s = 0
for i in range(1, n+1):
    s += i**2
```

For the specific sum (3.1) we just replace `i**2` by the right term inside the `for` loop:

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

Observe the factors `1.0` used to avoid integer division, since `i` is `int` and `x` may also be `int`.

It is natural to embed the computation of the sum in a function that takes x and n as arguments and returns the sum:

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

Our formula (3.1) is not chosen at random. In fact, it can be shown that $L(x;n)$ is an approximation to $\ln(1+x)$ for a finite n and $x \geq 1$. The approximation becomes exact in the limit

$$\lim_{n\to\infty} L(x;n) = \ln(1+x)\,.$$

Computational significance of $L(x;n)$

Although we can compute $\ln(1+x)$ on a calculator or by `math.log(1+x)` in Python, you may have wondered how such a function is actually calculated inside the calculator or the `math` module. In most cases this must be done via simple mathematical expressions such as the sum in (3.1). A calculator and the `math` module will use more sophisticated formulas than (3.1) for ultimate efficiency of the calculations, but the main point is that the numerical values of mathematical functions like $\ln(x)$, $\sin(x)$, and $\tan(x)$ are usually computed by sums similar to (3.1).

Instead of having our `L` function just returning the value of the sum, we could return additional information on the error involved in the approximation of $\ln(1+x)$ by $L(x;n)$. The size of the terms decreases with increasing n, and the first neglected term is then bigger than all the remaining terms, but not necessarily bigger than their sum. The first neglected term is hence an indication of the size of the total error we make, so we may use this term as a rough estimate of the error. For comparison, we could also return the exact error since we are able to calculate the ln function by `math.log`.

A new version of the `L(x, n)` function, where we return the value of $L(x;n)$, the first neglected term, and the exact error goes as follows:

```
def L2(x, n):
    s = 0
    for i in range(1, n+1):
        s += (1.0/i)*(x/(1.0+x))**i
    value_of_sum = s
    first_neglected_term = (1.0/(n+1))*(x/(1.0+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:
value, approximate_error, exact_error = L2(x, 100)
```

The next section demonstrates the usage of the `L2` function to judge the quality of the approximation $L(x;n)$ to $\ln(1+x)$.

3.1.9 Functions with no return values

Sometimes a function just performs a set of statements, without computing objects that are natural to return to the calling code. In such situations one can simply skip the `return` statement. Some programming

languages use the terms *procedure* or *subroutine* for functions that do not return anything.

Let us exemplify a function without return values by making a table of the accuracy of the $L(x;n)$ approximation to $\ln(1+x)$ from the previous section:

```
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)
```

This function just performs a set of statements that we may want to run several times. Calling

```
table(10)
table(1000)
```

gives the output

```
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)

x=1000, ln(1+x)=6.90875
n=1    0.999001    (next term: 4.99e-01  error: 5.91e+00)
n=2    1.498       (next term: 3.32e-01  error: 5.41e+00)
n=10   2.919       (next term: 8.99e-02  error: 3.99e+00)
n=100  5.08989     (next term: 8.95e-03  error: 1.82e+00)
n=500  6.34928     (next term: 1.21e-03  error: 5.59e-01)
```

From this output we see that the sum converges much more slowly when x is large than when x is small. We also see that the error is an order of magnitude or more larger than the first neglected term in the sum. The functions `L`, `L2`, and `table` are found in the file `lnsum.py`.

When there is no explicit `return` statement in a function, Python actually inserts an invisible `return None` statement. `None` is a special object in Python that represents something we might think of as empty data or just "nothing". Other computer languages, such as C, C++, and Java, use the word *void* for a similar thing. Normally, one will call the `table` function without assigning the return value to any variable, but if we assign the return value to a variable, `result = table(500)`, `result` will refer to a `None` object.

The `None` value is often used for variables that should exist in a program, but where it is natural to think of the value as conceptually undefined. The standard way to test if an object `obj` is set to `None` or not reads

```
if obj is None:
    ...
if obj is not None:
    ...
```

One can also use `obj == None`. The `is` operator tests if two names refer to the same object, while `==` tests if the contents of two objects are the same:

```
>>> a = 1
>>> b = a
>>> a is b   # a and b refer to the same object
True
>>> c = 1.0
>>> a is c
False
>>> a == c   # a and c are mathematically equal
True
```

3.1.10 Keyword arguments

Some function arguments can be given a default value so that we may leave out these arguments in the call. A typical function may look as

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

The first two arguments, `arg1` and `arg2`, are *ordinary* or *positional* arguments, while the latter two are *keyword arguments* or *named arguments*. Each keyword argument has a name (in this example `kwarg1` and `kwarg2`) and an associated default value. The keyword arguments must always be listed after the positional arguments in the function definition.

When calling `somefunc`, we may leave out some or all of the keyword arguments. Keyword arguments that do not appear in the call get their values from the specified default values. We can demonstrate the effect through some calls:

```
>>> somefunc('Hello', [1,2])
Hello [1, 2] True 0
>>> somefunc('Hello', [1,2], kwarg1='Hi')
Hello [1, 2] Hi 0
>>> somefunc('Hello', [1,2], kwarg2='Hi')
Hello [1, 2] True Hi
>>> somefunc('Hello', [1,2], kwarg2='Hi', kwarg1=6)
Hello [1, 2] 6 Hi
```

The sequence of the keyword arguments does not matter in the call. We may also mix the positional and keyword arguments if we explicitly write `name=value` for all arguments in the call:

```
>>> somefunc(kwarg2='Hello', arg1='Hi', kwarg1=6, arg2=[1,2],)
Hi [1, 2] 6 Hello
```

Example: Function with default parameters. Consider a function of t which also contains some parameters, here A, a, and ω:

$$f(t; A, a, \omega) = Ae^{-at}\sin(\omega t)\,. \tag{3.2}$$

We can implement f as a Python function where the independent variable t is an ordinary positional argument, and the parameters A, a, and ω are keyword arguments with suitable default values:

```
from math import pi, exp, sin

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

Calling `f` with just the `t` argument specified is possible:

```
v1 = f(0.2)
```

In this case we evaluate the expression $e^{-0.2}\sin(2\pi \cdot 0.2)$. Other possible calls include

```
v2 = f(0.2, omega=1)
v3 = f(1, A=5, omega=pi, a=pi**2)
v4 = f(A=5, a=2, t=0.01, omega=0.1)
v5 = f(0.2, 0.5, 1, 1)
```

You should write down the mathematical expressions that arise from these four calls. Also observe in the third line above that a positional argument, `t` in that case, can appear in between the keyword arguments if we write the positional argument on the keyword argument form `name=value`. In the last line we demonstrate that keyword arguments can be used as positional argument, i.e., the name part can be skipped, but then the sequence of the keyword arguments in the call must match the sequence in the function definition exactly.

Example: Computing a sum with default tolerance. Consider the $L(x; n)$ sum and the Python implementations `L(x, n)` and `L2(x, n)` from Section 3.1.8. Instead of specifying the number of terms in the sum, n, it is better to specify a tolerance ε of the accuracy. We can use the first neglected term as an estimate of the accuracy. This means that we sum up terms as long as the absolute value of the next term is greater than ϵ. It is natural to provide a default value for ϵ:

```
def L3(x, epsilon=1.0E-6):
    x = float(x)
    i = 1
    term = (1.0/i)*(x/(1+x))**i
    s = term
    while abs(term) > epsilon:
        i += 1
        term = (1.0/i)*(x/(1+x))**i
        s += term
    return s, i
```

Here is an example involving this function to make a table of the approximation error as ϵ decreases:

```
def table2(x):
    from math import log
    for k in range(4, 14, 2):
        epsilon = 10**(-k)
        approx, n = L3(x, epsilon=epsilon)
        exact = log(1+x)
        exact_error = exact - approx
```

The output from calling `table2(10)` becomes

```
epsilon: 1e-04, exact error: 8.18e-04, n=55
epsilon: 1e-06, exact error: 9.02e-06, n=97
epsilon: 1e-08, exact error: 8.70e-08, n=142
epsilon: 1e-10, exact error: 9.20e-10, n=187
epsilon: 1e-12, exact error: 9.31e-12, n=233
```

We see that the `epsilon` estimate is almost 10 times smaller than the exact error, regardless of the size of `epsilon`. Since `epsilon` follows the exact error quite well over many orders of magnitude, we may view `epsilon` as a useful indication of the size of the error.

3.1.11 Doc strings

There is a convention in Python to insert a documentation string right after the `def` line of the function definition. The documentation string, known as a *doc string*, should contain a short description of the purpose of the function and explain what the different arguments and return values are. Interactive sessions from a Python shell are also common to illustrate how the code is used. Doc strings are usually enclosed in triple double quotes `"""`, which allow the string to span several lines.

Here are two examples on short and long doc strings:

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

Note that the doc string must appear before any statement in the function body.

There are several Python tools that can automatically extract doc strings from the source code and produce various types of documentation. The leading tools is Sphinx[3], see also [13, Appendix B.2].

[3] `http://sphinx-doc.org/invocation.html#invocation-apidoc`

The doc string can be accessed in a code as `funcname.__doc__`, where `funcname` is the name of the function, e.g.,

```
print line.__doc__
```

which prints out the documentation of the `line` function above:

```
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 (float objects).
x1, y1: another point on the line (float objects).
return: coefficients a, b for the line (y=a*x+b).
```

If the function `line` is in a file `funcs.py`, we may also run `pydoc funcs.line` in a terminal window to look the documentation of the `line` function in terms of the function signature and the doc string.

Doc strings often contain interactive sessions, copied from a Python shell, to illustrate how the function is used. We can add such a session to the doc string in the `line` function:

```
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 (float).
    x1, y1: another point on the line (float).
    return: coefficients a, b (floats) for the line (y=a*x+b).

    Example:
    >>> a, b = line(1, -1, 4, 3)
    >>> a
    1.3333333333333333
    >>> b
    -2.333333333333333
    """
    a = (y1 - y0)/float(x1 - x0)
    b = y0 - a*x0
    return a, b
```

A particularly nice feature is that all such interactive sessions in doc strings can be automatically run, and new results are compared to the results found in the doc strings. This makes it possible to use interactive sessions in doc strings both for exemplifying how the code is used and for testing that the code works.

Function input and output

It is a convention in Python that function arguments represent the input data to the function, while the returned objects represent the output data. We can sketch a general Python function as

```
def somefunc(i1, i2, i3, io4, io5, i6=value1, io7=value2):
    # modify io4, io5, io6; compute o1, o2, o3
    return o1, o2, o3, io4, io5, io7
```

Here `i1`, `i2`, `i3` are positional arguments representing input data; `io4` and `io5` are positional arguments representing input *and* output data; `i6` and `io7` are keyword arguments representing input and input/output data, respectively; and `o1`, `o2`, and `o3` are computed objects in the function, representing output data together with `io4`, `io5`, and `io7`. All examples later in the book will make use of this convention.

3.1.12 Functions as arguments to functions

Programs doing calculus frequently need to have functions as arguments in functions. For example, a mathematical function $f(x)$ is needed in Python functions for

- numerical root finding: solve $f(x) = 0$ approximately (Sections 4.10.2 and A.1.10)
- numerical differentiation: compute $f'(x)$ approximately (Sections B.2 and 7.3.2)
- numerical integration: compute $\int_a^b f(x)dx$ approximately (Sections B.3 and 7.3.3)
- numerical solution of differential equations: $\frac{dx}{dt} = f(x)$ (Appendix E)

In such Python functions we need to have the $f(x)$ function as an argument `f`. This is straightforward in Python and hardly needs any explanation, but in most other languages special constructions must be used for transferring a function to another function as argument.

As an example, consider a function for computing the second-order derivative of a function $f(x)$ numerically:

$$f''(x) \approx \frac{f(x-h) - 2f(x) + f(x+h)}{h^2}, \tag{3.3}$$

where h is a small number. The approximation (3.3) becomes exact in the limit $h \to 0$. A Python function for computing (3.3) can be implemented as follows:

```
def diff2nd(f, x, h=1E-6):
    r = (f(x-h) - 2*f(x) + f(x+h))/float(h*h)
    return r
```

The `f` argument is like any other argument, i.e., a name for an object, here a function object that we can call as we normally call functions. An application of `diff2nd` may be

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

t = 1.2
d2g = diff2nd(g, t)
print "g''(%f)=%f" % (t, d2g)
```

The behavior of the numerical derivative as $h \to 0$. From mathematics we know that the approximation formula (3.3) becomes more accurate as h decreases. Let us try to demonstrate this expected feature by making a table of the second-order derivative of $g(t) = t^{-6}$ at $t = 1$ as $h \to 0$:

```
for k in range(1,15):
    h = 10**(-k)
    d2g = diff2nd(g, 1, h)
    print 'h=%.0e: %.5f' % (h, d2g)
```

The output becomes

```
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
```

With $g(t) = t^{-6}$, the exact answer is $g''(1) = 42$, but for $h < 10^{-8}$ the computations give totally wrong answers! The problem is that for small h on a computer, round-off errors in the formula (3.3) blow up and destroy the accuracy. The mathematical result that (3.3) becomes an increasingly better approximation as h gets smaller and smaller does not hold on a computer! Or more precisely, the result holds until h in the present case reaches 10^{-4}.

The reason for the inaccuracy is that the numerator in (3.3) for $g(t) = t^{-6}$ and $t = 1$ contains subtraction of quantities that are almost equal. The result is a very small and inaccurate number. The inaccuracy is magnified by h^{-2}, a number that becomes very large for small h.

Switching from the standard floating-point numbers (`float`) to numbers with arbitrary high precision resolves the problem. Python has a module `decimal` that can be used for this purpose. The file `high_precision.py` solves the current problem using arithmetics based on the `decimal` module. With 25 digits in `x` and `h` inside the `diff2nd` function, we get accurate results for $h \leq 10^{-13}$. However, for most practical applications of (3.3), a moderately small h, say $10^{-3} \leq h \leq 10^{-4}$, gives sufficient accuracy and then round-off errors from `float` calculations do not pose problems. Real-world science or engineering applications usually have many parameters with uncertainty, making the end result also

uncertain, and formulas like (3.3) can then be computed with moderate accuracy without affecting the overall uncertainty in the answers.

3.1.13 The main program

In programs containing functions we often refer to a part of the program that is called the *main program*. This is the collection of all the statements outside the functions, plus the definition of all functions. Let us look at a complete program:

```
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 main program here consists of the lines with a comment `in main`. The execution always starts with the first line in the main program. When a function is encountered, its statements are just used to define the function - nothing gets computed inside the function before we explicitly call the function, either from the main program or from another function. All variables initialized in the main program become global variables (see Section 3.1.3).

The program flow in the program above goes as follows:

- Import functions from the `math` module,
- define a function `f(x)`,
- define `x`,
- call `f` and execute the function body,
- define `y` as the value returned from `f`,
- print the string.

In point 4, we jump to the `f` function and execute the statement inside that function for the first time. Then we jump back to the main program and assign the `float` object returned from `f` to the `y` variable.

Readers who are uncertain about the program flow and the jumps between the main program and functions should use a debugger or the Online Python Tutor as explained in Section 3.1.2.

3.1.14 Lambda functions

There is a quick one-line construction of functions that is often convenient to make Python code compact:

```
f = lambda x: x**2 + 4
```

This so-called *lambda function* is equivalent to writing

```
def f(x):
    return x**2 + 4
```

In general,

```
def g(arg1, arg2, arg3, ...):
    return expression
```

can be written as

```
g = lambda arg1, arg2, arg3, ...: expression
```

Lambda functions are usually used to quickly define a function as argument to another function. Consider, as an example, the `diff2nd` function from Section 3.1.12. In the example from that chapter we want to differentiate $g(t) = t^{-6}$ twice and first make a Python function `g(t)` and then send this `g` to `diff2nd` as argument. We can skip the step with defining the `g(t)` function and instead insert a lambda function as the `f` argument in the call to `diff2nd`:

```
d2 = diff2nd(lambda t: t**(-6), 1, h=1E-4)
```

Because lambda functions saves quite some typing, at least for very small functions, they are popular among many programmers.

Lambda functions may also take keyword arguments. For example,

```
d2 = diff2nd(lambda t, A=1, a=0.5: -a*2*t*A*exp(-a*t**2), 1.2)
```

3.2 Branching

The flow of computer programs often needs to branch. That is, if a condition is met, we do one thing, and if not, we do another thing. A simple example is a function defined as

$$f(x) = \begin{cases} \sin x, & 0 \leq x \leq \pi \\ 0, & \text{otherwise} \end{cases} \tag{3.4}$$

In a Python implementation of this function we need to test on the value of x, which can be done as displayed below:

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

3.2.1 If-else blocks

The general structure of an `if-else` test is

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

When `condition` evaluates to `True`, the program flow branches into the first block of statements. If `condition` is `False`, the program flow jumps to the second block of statements, after the `else:` line. As with `while` and `for` loops, the block of statements are indented. Here is another example:

```
if C < -273.15:
    print '%g degrees Celsius is non-physical!' % C
    print 'The Fahrenheit temperature will not be computed.'
else:
    F = 9.0/5*C + 32
    print F
print 'end of program'
```

The two `print` statements in the `if` block are executed if and only if `C < -273.15` evaluates to `True`. Otherwise, we jump over the first two `print` statements and carry out the computation and printing of `F`. The printout of `end of program` will be performed regardless of the outcome of the `if` test since this statement is not indented and hence neither a part of the `if` block nor the `else` block.

The `else` part of an `if` test can be skipped, if desired:

```
if condition:
    <block of statements>
<next statement>
```

For example,

```
if C < -273.15:
    print '%s degrees Celsius is non-physical!' % C
F = 9.0/5*C + 32
```

In this case the computation of `F` will always be carried out, since the statement is not indented and hence not a part of the `if` block.

With the keyword `elif`, short for *else if*, we can have several mutually exclusive `if` tests, which allows for multiple branching of the program flow:

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

The last `else` part can be skipped if it is not needed. To illustrate multiple branching we will implement a *hat function*, which is widely used in advanced computer simulations in science and industry. One example of a hat function is

$$N(x) = \begin{cases} 0, & x < 0 \\ x, & 0 \leq x < 1 \\ 2 - x, & 1 \leq x < 2 \\ 0, & x \geq 2 \end{cases} \tag{3.5}$$

The solid line in Figure 5.9 in Section 5.4.1 illustrates the shape of this function and why it is called a hat function. The Python implementation associated with (3.5) needs multiple `if` branches:

```
def N(x):
    if x < 0:
        return 0.0
    elif 0 <= x < 1:
        return x
    elif 1 <= x < 2:
        return 2 - x
    elif x >= 2:
        return 0.0
```

This code corresponds directly to the mathematical specification, which is a sound strategy that help reduce the amount of errors in programs. We could mention that there is another way of constructing the `if` test that results in shorter code:

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

As a part of learning to program, understanding this latter sample code is important, but we recommend the former solution because of its direct similarity with the mathematical definition of the function.

A popular programming rule is to avoid multiple `return` statements in a function - there should only be one `return` at the end. We can do that in the `N` function by introducing a local variable, assigning values to this variable in the blocks and returning the variable at the end. However, we do not think an extra variable and an extra line make a great improvement in such a short function. Nevertheless, in long and complicated functions the rule can be helpful.

3.2.2 Inline if tests

A variable is often assigned a value that depends on a boolean expression. This can be coded using a common `if-else` test:

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

Because this construction is often needed, Python provides a one-line syntax for the four lines above:

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

The parentheses are not required, but recommended style. One example is

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

Since the inline `if` test is an expression with a value, it can be used in lambda functions:

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

The traditional `if-else` construction with indented blocks cannot be used inside lambda functions because it is not just an expression (lambda functions cannot have statements inside them, only a single expression).

3.3 Mixing loops, branching, and functions in bioinformatics examples

Life is definitely digital. The genetic code of all living organisms are represented by a long sequence of simple molecules called nucleotides, or bases, which makes up the Deoxyribonucleic acid, better known as DNA. There are only four such nucleotides, and the entire genetic code of a human can be seen as a simple, though 3 billion long, string of the letters A, C, G, and T. Analyzing DNA data to gain increased biological understanding is much about searching in long strings for certain string patterns involving the letters A, C, G, and T. This is an integral part of *bioinformatics*, a scientific discipline addressing the use of computers to search for, explore, and use information about genes, nucleic acids, and proteins.

The leading Python software for bioinformatics applications is BioPython[4]. The examples in this book (below and Sections 6.5, 8.3.4, and 9.5) are simple illustrations of the type of problem settings and corresponding Python implementations that are encountered in bioinformatics. For real-world problem solving one should rather utilize BioPython, but the sections below act as an introduction to what is inside packages like BioPython.

[4] `http://biopython.org`

We start with some very simple examples on DNA analysis that bring together basic building blocks in programming: loops, `if` tests, and functions.

3.3.1 Counting letters in DNA strings

Given some string `dna` containing the letters A, C, G, or T, representing the bases that make up DNA, we ask the question: how many times does a certain base occur in the DNA string? For example, if `dna` is ATGGCATTA and we ask how many times the base A occur in this string, the answer is 3.

A general Python implementation answering this problem can be done in many ways. Several possible solutions are presented below.

List iteration. The most straightforward solution is to loop over the letters in the string, test if the current letter equals the desired one, and if so, increase a counter. Looping over the letters is obvious if the letters are stored in a list. This is easily done by converting a string to a list:

```
>>> list('ATGC')
['A', 'T', 'G', 'C']
```

Our first solution becomes

```
def count_v1(dna, base):
    dna = list(dna)  # convert string to list of letters
    i = 0            # counter
    for c in dna:
        if c == base:
            i += 1
    return i
```

String iteration. Python allows us to iterate directly over a string without converting it to a list:

```
>>> for c in 'ATGC':
...     print c
A
T
G
C
```

In fact, all built-in objects in Python that contain a set of elements in a particular sequence allow a `for` loop construction of the type `for element in object`.

A slight improvement of our solution is therefore to iterate directly over the string:

```
def count_v2(dna, base):
    i = 0 # counter
    for c in dna:
        if c == base:
```

```
            i += 1
    return i

dna = 'ATGCGGACCTAT'
base = 'C'
n = count_v2(dna, base)

# printf-style formatting
print '%s appears %d times in %s' % (base, n, dna)

# or (new) format string syntax
print '{base} appears {n} times in {dna}'.format(
    base=base, n=n, dna=dna)
```

We have here illustrated two alternative ways of writing out text where the value of variables are to be inserted in "slots" in the string.

Index iteration. Although it is natural in Python to iterate over the letters in a string (or more generally over elements in a sequence), programmers with experience from other languages (Fortran, C and Java are examples) are used to `for` loops with an integer counter running over all indices in a string or array:

```
def count_v3(dna, base):
    i = 0 # counter
    for j in range(len(dna)):
        if dna[j] == base:
            i += 1
    return i
```

Python indices always start at 0 so the legal indices for our string become `0`, `1`, ..., `len(dna)-1`, where `len(dna)` is the number of letters in the string `dna`. The `range(x)` function returns a list of integers `0`, `1`, ..., `x-1`, implying that `range(len(dna))` generates all the legal indices for `dna`.

While loops. The `while` loop equivalent to the last function reads

```
def count_v4(dna, base):
    i = 0 # counter
    j = 0 # string index
    while j < len(dna):
        if dna[j] == base:
            i += 1
        j += 1
    return i
```

Correct indentation is here crucial: a typical error is to fail indenting the `j += 1` line correctly.

Summing a boolean list. The idea now is to create a list `m` where `m[i]` is `True` if `dna[i]` equals the letter we search for (`base`). The number of `True` values in `m` is then the number of `base` letters in `dna`. We can use the `sum` function to find this number because doing arithmetics with boolean lists automatically interprets `True` as `1` and `False` as `0`. That is, `sum(m)` returns the number of `True` elements in `m`. A possible function doing this is

```
def count_v5(dna, base):
    m = []   # matches for base in dna: m[i]=True if dna[i]==base
    for c in dna:
        if c == base:
            m.append(True)
        else:
            m.append(False)
    return sum(m)
```

Inline if test. Shorter, more compact code is often a goal if the compactness enhances readability. The four-line `if` test in the previous function can be condensed to one line using the inline `if` construction: `if condition value1 else value2`.

```
def count_v6(dna, base):
    m = []   # matches for base in dna: m[i]=True if dna[i]==base
    for c in dna:
        m.append(True if c == base else False)
    return sum(m)
```

Using boolean values directly. The inline `if` test is in fact redundant in the previous function because the value of the condition `c == base` can be used directly: it has the value `True` or `False`. This saves some typing and adds clarity, at least to Python programmers with some experience:

```
def count_v7(dna, base):
    m = []   # matches for base in dna: m[i]=True if dna[i]==base
    for c in dna:
        m.append(c == base)
    return sum(m)
```

List comprehensions. Building a list with the aid of a `for` loop can often be condensed to a single line by using list comprehensions: `[expr for e in sequence]`, where `expr` is some expression normally involving the iteration variable `e`. In our last example, we can introduce a list comprehension

```
def count_v8(dna, base):
    m = [c == base for c in dna]
    return sum(m)
```

Here it is tempting to get rid of the `m` variable and reduce the function body to a single line:

```
def count_v9(dna, base):
    return sum([c == base for c in dna])
```

Using a sum iterator. The DNA string is usually huge - 3 billion letters for the human species. Making a boolean array with `True` and `False` values therefore increases the memory usage by a factor of two in our sample functions `count_v5` to `count_v9`. Summing without actually storing an extra list is desirable. Fortunately, `sum([x for x in s])` can

be replaced by `sum(x for x in s)`, where the latter sums the elements in `s` as `x` visits the elements of `s` one by one. Removing the brackets therefore avoids first making a list before applying `sum` to that list. This is a minor modification of the `count_v9` function:

```
def count_v10(dna, base):
    return sum(c == base for c in dna)
```

Below we shall measure the impact of the various program constructs on the CPU time.

Extracting indices. Instead of making a boolean list with elements expressing whether a letter matches the given `base` or not, we may collect all the indices of the matches. This can be done by adding an `if` test to the list comprehension:

```
def count_v11(dna, base):
    return len([i for i in range(len(dna)) if dna[i] == base])
```

The Online Python Tutor[5] is really helpful to reach an understanding of this compact code. Alternatively, you may play with the constructions in an interactive Python shell:

```
>>> dna = 'AATGCTTA'
>>> base = 'A'
>>> indices = [i for i in range(len(dna)) if dna[i] == base]
>>> indices
[0, 1, 7]
>>> print dna[0], dna[1], dna[7]  # check
A A A
```

Observe that the element `i` in the list comprehension is only made for those `i` where `dna[i] == base`.

Using Python's library. Very often when you set out to do a task in Python, there is already functionality for the task in the object itself, in the Python libraries, or in third-party libraries found on the Internet. Counting how many times a letter (or substring) `base` appears in a string `dna` is obviously a very common task so Python supports it by the syntax `dna.count(base)`:

```
def count_v12(dna, base):
    return dna.count(base)

def compare_efficiency():
```

3.3.2 Efficiency assessment

Now we have 11 different versions of how to count the occurrences of a letter in a string. Which one of these implementations is the fastest?

[5] `http://www.pythontutor.com/`

To answer the question we need some test data, which should be a huge string `dna`.

Generating random DNA strings. The simplest way of generating a long string is to repeat a character a large number of times:

```
N = 1000000
dna = 'A'*N
```

The resulting string is just `'AAA...A`, of length `N`, which is fine for testing the efficiency of Python functions. Nevertheless, it is more exciting to work with a DNA string with letters from the whole alphabet A, C, G, and T. To make a DNA string with a random composition of the letters we can first make a list of random letters and then join all those letters to a string:

```
import random
alphabet = list('ATGC')
dna = [random.choice(alphabet) for i in range(N)]
dna = ''.join(dna)  # join the list elements to a string
```

The `random.choice(x)` function selects an element in the list `x` at random.

Note that `N` is very often a large number. In Python version 2.x, `range(N)` generates a list of `N` integers. We can avoid the list by using `xrange` which generates an integer at a time and not the whole list. In Python version 3.x, the `range` function is actually the `xrange` function in version 2.x. Using `xrange`, combining the statements, and wrapping the construction of a random DNA string in a function, gives

```
import random

def generate_string(N, alphabet='ACGT'):
    return ''.join([random.choice(alphabet) for i in xrange(N)])

dna = generate_string(600000)
```

The call `generate_string(10)` may generate something like `AATGGCAGAA`.

Measuring CPU time. Our next goal is to see how much time the various `count_v*` functions spend on counting letters in a huge string, which is to be generated as shown above. Measuring the time spent in a program can be done by the `time` module:

```
import time
...
t0 = time.clock()
# do stuff
t1 = time.clock()
cpu_time = t1 - t0
```

The `time.clock()` function returns the CPU time spent in the program since its start. If the interest is in the total time, also including reading and writing files, `time.time()` is the appropriate function to call.

Running through all our functions made so far and recording timings can be done by

```
import time
functions = [count_v1, count_v2, count_v3, count_v4,
             count_v5, count_v6, count_v7, count_v8,
             count_v9, count_v10, count_v11, count_v12]
timings = []  # timings[i] holds CPU time for functions[i]

for function in functions:
    t0 = time.clock()
    function(dna, 'A')
    t1 = time.clock()
    cpu_time = t1 - t0
    timings.append(cpu_time)
```

In Python, functions are ordinary objects so making a list of functions is no more special than making a list of strings or numbers.

We can now iterate over `timings` and `functions` simultaneously via `zip` to make a nice printout of the results:

```
for cpu_time, function in zip(timings, functions):
    print '{f:<9s}: {cpu:.2f} s'.format(
        f=function.func_name, cpu=cpu_time)
```

Timings on a MacBook Air 11 running Ubuntu show that the functions using `list.append` require almost the double of the time of the functions that work with list comprehensions. Even faster is the simple iteration over the string. However, the built-in count functionality of strings (`dna.count(base)`) runs over 30 times faster than the best of our handwritten Python functions! The reason is that the `for` loop needed to count in `dna.count(base)` is actually implemented in C and runs very much faster than loops in Python.

A clear lesson learned is: google around before you start out to implement what seems to be a quite common task. Others have probably already done it for you, and most likely is their solution much better than what you can (easily) come up with.

3.3.3 Verifying the implementations

We end this section with showing how to make tests that verify our 12 counting functions. To this end, we make a new function that first computes a certainly correct answer to a counting problem and then calls all the `count_*` functions, stored in the list `functions`, to check that each call has the correct result:

```
def test_count_all():
    dna = 'ATTTGCGGTCCAAA'
    exact = dna.count('A')
    for f in functions:
        if f(dna, 'A') != exact:
            print f.__name__, 'failed'
```

Here, we believe in `dna.count('A')` as the correct answer.

We might take this test function one step further and adopt the conventions in the pytest[6] and nose[7] testing frameworks for Python code. (See Section H.6 for more information about pytest and nose.)

These conventions say that the test function should

- have a name starting with `test_`;
- have no arguments;
- let a boolean variable, say `success`, be `True` if a test passes and be `False` if the test fails;
- create a message about what failed, stored in some string, say `msg`;
- use the construction `assert success, msg`, which will abort the program and write out the error message `msg` if `success` is `False`.

The pytest and nose test frameworks can search for all Python files in a folder tree, run all `test_*()` functions, and report how many of the tests that failed, if we adopt the conventions above. Our revised test function becomes

```
def test_count_all():
    dna = 'ATTTGCGGTCCAAA'
    exact = dna.count('A')
    for f in functions:
        success = f(dna, 'A') == exact
        msg = '%s failed' % f.__name__
        assert success, msg
```

It is worth notifying that the name of a function `f`, as a string object, is given by `f.__name__`, and we make use of this information to construct an informative message in case a test fails.

It is a good habit to write such test functions since the execution of all tests in all files can be fully automated. Every time you to a change in some file you can with minimum effort rerun all tests.

The entire suite of functions presented above, including the timings and tests, can be found in the file `count.py`.

3.4 Summary

3.4.1 Chapter topics

User-defined functions. Functions are useful (i) when a set of commands are to be executed several times, or (ii) to partition the program into smaller pieces to gain better overview. Function arguments are local variables inside the function whose values are set when calling the function. Remember that when you write the function, the values of the arguments

[6] `http://pytest.org`
[7] `https://nose.readthedocs.org`

are not known. Here is an example of a function for polynomials of 2nd degree:

```
# function definition:
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)
```

The sequence of the arguments is important, unless all arguments are given as `name=value`.

Functions may have no arguments and/or no return value(s):

```
def print_date():
    """Print the current date in the format 'Jan 07, 2007'."""
    import time
    print time.strftime("%b %d, %Y")

# call:
print_date()
```

A common error is to forget the parentheses: `print_date` is the function object itself, while `print_date()` is a call to the function.

Keyword arguments. Function arguments with default values are called keyword arguments, and they help to document the meaning of arguments in function calls. They also make it possible to specify just a subset of the arguments in function calls.

```
from math import exp, sin, pi

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

f1 = f(0)
x2 = 0.1
f2 = f(x2, w=2*pi)
f3 = f(x2, w=4*pi, A=10, a=0.1)
f4 = f(w=4*pi, A=10, a=0.1, x=x2)
```

The sequence of the keyword arguments can be arbitrary, and the keyword arguments that are not listed in the call get their default values according to the function definition. The non-keyword arguments are called positional arguments, which is `x` in this example. Positional arguments must be listed before the keyword arguments. However, also a positional argument can appear as `name=value` in the call (see the last line above), and this syntax allows any positional argument to be listed anywhere in the call.

If tests. The `if-elif-else` tests are used to *branch* the flow of statements. That is, different sets of statements are executed depending on whether some conditions are `True` or `False`.

```
def f(x):
    if x < 0:
        value = -1
    elif x >= 0 and x <= 1:
        value = x
    else:
        value = 1
    return value
```

Inline if tests. Assigning a variable one value if a condition is `True` and another value if `False`, is compactly done with an inline `if` test:

```
sign = -1 if a < 0 else 1
```

Terminology. The important computer science terms in this chapter are

- function
- method
- return statement
- positional arguments
- keyword arguments
- local and global variables
- doc strings
- `if` tests with `if`, `elif`, and `else` (branching)
- the `None` object
- test functions (for verification)

3.4.2 Example: Numerical integration

Problem. An integral

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

can be approximated by the so-called Simpson's rule:

$$\frac{b-a}{3n}\left(f(a)+f(b)+4\sum_{i=1}^{n/2}f(a+(2i-1)h)+2\sum_{i=1}^{n/2-1}f(a+2ih)\right). \tag{3.6}$$

Here, $h=(b-a)/n$ and n must be an even integer. The problem is to make a function `Simpson(f, a, b, n=500)` that returns the right-hand side formula of (3.6). To verify the implementation, one can make use of the fact that Simpson's rule is *exact* for all polynomials $f(x)$ of degree ≤ 2. Apply the `Simpson` function to the integral $\frac{3}{2}\int_0^\pi \sin^3 x dx$, which has exact value 2, and investigate how the approximation error varies with n.

Solution. The evaluation of the formula (3.6) in a program is straightforward if we know how to implement summation ($\sum$) and how to call f. A Python recipe for calculating sums is given in Section 3.1.8. Basically, $\sum_{i=M}^{N} q(i)$, for some expression $q(i)$ involving i, is coded with the aid of a `for` loop over i and an accumulation variable `s` for building up the sum, one term at a time:

```
s = 0
for i in range(M, N):
    s += q(i)
```

The `Simpson` function can then be coded as

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

Note that `Simpson` can integrate any Python function `f` of one variable. Specifically, we can implement

$$h(x) = \frac{3}{2}\sin^3 x dx$$

in a Python function

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

and call `Simpson` to compute $\int_0^\pi h(x)dx$ for various choices of n, as requested:

```
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)
```

(We have put the statements inside a function, here called `application`, mainly to group them, and not because `application` will be called several times or with different arguments.)

Verification. Calling `application()` leads to the output

```
Integral of 1.5*sin^3 from 0 to pi:
n=  2, approx= 3.141592653589793, error=-1.14E+00
n=  6, approx= 1.989171700583579, error= 1.08E-02
n= 12, approx= 1.999489233010781, error= 5.11E-04
```

```
n=100, approx= 1.999999902476350, error= 9.75E-08
n=500, approx= 1.999999999844138, error= 1.56E-10
```

We clearly see that the approximation improves as n increases. However, every computation will give an answer that deviates from the exact value 2. We cannot from this test alone know if the errors above are those implied by the approximation only, or if there are additional programming mistakes.

A much better way of verifying the implementation is therefore to look for test cases where the numerical approximation formula is *exact*, such that we know exactly what the result of the function should be. Since it is stated that the formula is exact for polynomials up to second degree, we just test the `Simpson` function on an "arbitrary" parabola, say

$$\int_{3/2}^{2} \left(3x^2 - 7x + 2.5\right) dx\,.$$

This integral equals $G(2) - G(3/2)$, where $G(x) = x^3 - 3.5x^2 + 2.5x$. A possible implementation becomes

```
def g(x):
    return 3*x**2 - 7*x + 2.5

def G(x):
    return x**3 - 3.5*x**2 + 2.5*x

def test_Simpson():
    a = 1.5
    b = 2.0
    n = 8
    exact = G(b) - G(a)
    approx = Simpson(g, a, b, n)
    success = abs(exact - approx) < 1E-14
    if not success:
        print 'Error: cannot integrate a quadratic function exactly'
```

Observe that we avoid testing `exact == approx` because there may be small round-off errors in these `float` objects so that the exact `==` test fails. Testing that the two variables are very close (distance less than 10^{-14}) is the rule of thumb for comparing `float` objects.

The `g` and `G` functions are only of interest inside the `test_Simpson` function. Many think the code becomes easier to read and understand if `g` and `G` are moved inside `test_Simpson`, which is indeed possible in Python:

```
def test_Simpson():
    def g(x):
        # test function that Simpson's rule will integrat exactly
        return 3*x**2 - 7*x + 2.5

    def G(x):
        # integral of g(x)
        return x**3 - 3.5*x**2 + 2.5*x

    a = 1.5
    b = 2.0
```

```
    n = 8
    exact = G(b) - G(a)
    approx = Simpson(g, a, b, n)
    success = abs(exact - approx) < 1E-14
    if not success:
        print 'Error: cannot integrate a quadratic function exactly'
```

We shall make it a habit to write functions like `test_Simpson` for verifying implementations. As was mentioned in Section 3.3.3, it can be wise to write our test function according to the conventions needed for applying the pytest and nose testing frameworks (Section H.6). Our pytest/nose-compatible test function then looks as follows:

```
def test_Simpson():
    """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  # never use == for floats!
    msg = 'Cannot integrate a quadratic function exactly'
    assert success, msg
```

Here we have also made the test function more compact by utilizing lambda functions for `g` and `G` (see Section 3.1.14).

Checking the validity of function arguments. Another improvement is to increase the robustness of the function. That is, to check that the input data, i.e., the arguments, are acceptable. Here we may test if $b > a$ and if n is an even integer. For the latter test, we make use of the *mod* function: mod(n, d) gives the remainder when n is divided by d (both n and d are integers). Mathematically, if p is the largest integer such that $pd \leq n$, then mod(n, d) is $n - pd$. For example, mod(3, 2) is 1, mod(3, 1) is 0, mod (3, 3) is 0, and mod(18, 8) is 2. The point is that n divided by d is an integer when mod(n, d) is zero. In Python, the percentage sign is used for the mod function:

```
>>> 18 % 8
2
```

To test if `n` is an odd integer, we see if it can be divided by 2 and yield an integer without any reminder: `n % 2 == 0`.

The improved `Simpson` function with validity tests on the provided arguments, as well as a doc string (Section 3.1.11), can look like this:

```
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.
    """
    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

    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 complete code is found in the file `Simpson.py`.

A very good exercise is to simulate the program flow by hand, starting with the call to the `application` function. The Online Python Tutor or a debugger (see Section F.1) are convenient tools for controlling that your thinking is correct.

3.5 Exercises

Exercise 3.1: Write a Fahrenheit-Celsius conversion function

The formula for converting Fahrenheit degrees to Celsius reads

$$C = \frac{5}{9}(F - 32)\,. \tag{3.7}$$

Write a function `C(F)` that implements this formula. To verify the implementation, you can use `F(C)` from Section 3.1.1 and test that `C(F(c)` equals `c`.

Hint. Do not test `C(F(c)) == c` exactly, but use a tolerance for the difference.
Filename: `f2c.py`.

Exercise 3.2: Evaluate a sum and write a test function

a) Write a Python function `sum_1k(M)` that returns the sum $s = \sum_{k=1}^{M} \frac{1}{k}$.

b) Compute s for $M = 3$ by hand and write another function `test_sum_1k()` that calls `sum_1k(3)` and checks that the answer is correct.

Hint. We recommend that `test_sum_1k` follows the conventions of the pytest and nose testing frameworks as explained in Sections 3.3.3 and 3.4.2 (see also Section H.6). It means setting a boolean variable `success` to

`True` if the test passes, otherwise `False`. The next step is to do `assert success`, which will abort the program with an error message if `success` is `False` and the test failed. To provide an informative error message, you can add your own message string `msg`: `assert success, msg`.
Filename: `sum_func.py`.

Exercise 3.3: Write a function for solving $ax^2 + bx + c = 0$

a) Given a quadratic equation $ax^2+bx+c = 0$, write a function `roots(a, b, c)` that returns the two roots of the equation. The returned roots should be `float` objects when the roots are real, otherwise the function returns `complex` objects.

Hint. Use `sqrt` from the `numpy.lib.scimath` library, see Chapter 1.6.3.

b) Construct two test cases with known solutions, one with real roots and the other with complex roots, Implement the two test cases in two test functions `test_roots_float` and `test_roots_complex`, where you call the `roots` function and check the type and value of the returned objects.
Filename: `roots_quadratic.py`.

Exercise 3.4: Implement the sum function

The standard Python function called `sum` takes a list as argument and computes the sum of the elements in the list:

```
>>> sum([1,3,5,-5])
4
>>> sum([[1,2], [4,3], [8,1]])
[1, 2, 4, 3, 8, 1]
>>> sum(['Hello, ', 'World!'])
'Hello, World!'
```

Implement your own version of `sum`. Filename: `mysum.py`.

Exercise 3.5: Compute a polynomial via a product

Given $n+1$ roots $r_0, r_1, \ldots, r_n$ of a polynomial $p(x)$ of degree $n+1$, $p(x)$ can be computed by

$$p(x) = \prod_{i=0}^{n}(x - r_i) = (x - r_0)(x - r_1)\cdots(x - r_{n-1})(x - r_n)\,. \qquad (3.8)$$

Write a function `poly(x, roots)` that takes x and a list `roots` of the roots as arguments and returns $p(x)$. Construct a test case for verifying the implementation. Filename: `polyprod.py`.

Exercise 3.6: Integrate a function by the Trapezoidal rule

a) An approximation to the integral of a function $f(x)$ over an interval $[a, b]$ can be found by first approximating $f(x)$ by the straight line that goes through the end points $(a, f(a))$ and $(b, f(b))$, and then finding the area under the straight line, which is the area of a trapezoid. The resulting formula becomes

$$\int_a^b f(x)dx \approx \frac{b-a}{2}(f(a) + f(b)) \,. \tag{3.9}$$

Write a function `trapezint1(f, a, b)` that returns this approximation to the integral. The argument `f` is a Python implementation `f(x)` of the mathematical function $f(x)$.

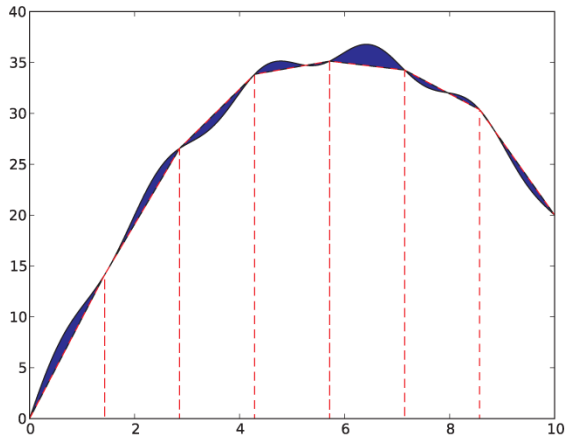
b) Use the approximation (3.9) to compute the following integrals: $\int_0^\pi \cos x \, dx$, $\int_0^\pi \sin x \, dx$, and $\int_0^{\pi/2} \sin x \, dx$, In each case, write out the error, i.e., the difference between the exact integral and the approximation (3.9). Make rough sketches of the trapezoid for each integral in order to understand how the method behaves in the different cases.

c) We can easily improve the formula (3.9) by approximating the area under the function $f(x)$ by two equal-sized trapezoids. Derive a formula for this approximation and implement it in a function `trapezint2(f, a, b)`. Run the examples from b) and see how much better the new formula is. Make sketches of the two trapezoids in each case.

d) A further improvement of the approximate integration method from c) is to divide the area under the $f(x)$ curve into n equal-sized trapezoids. Based on this idea, derive the following formula for approximating the integral:

$$\int_a^b f(x)dx \approx \sum_{0=1}^{n-1} \frac{1}{2} h \left(f(x_i) + f(x_{i+1})\right) , \tag{3.10}$$

where h is the width of the trapezoids, $h = (b-a)/n$, and $x_i = a + ih$, $i = 0, \ldots, n$, are the coordinates of the sides of the trapezoids. The figure below visualizes the idea of the Trapezoidal rule.



Implement (3.10) in a Python function `trapezint(f, a, b, n)`. Run the examples from b) with $n = 10$.

e) Write a test function `test_trapezint()` for verifying the implementation of the function `trapezint` in d).

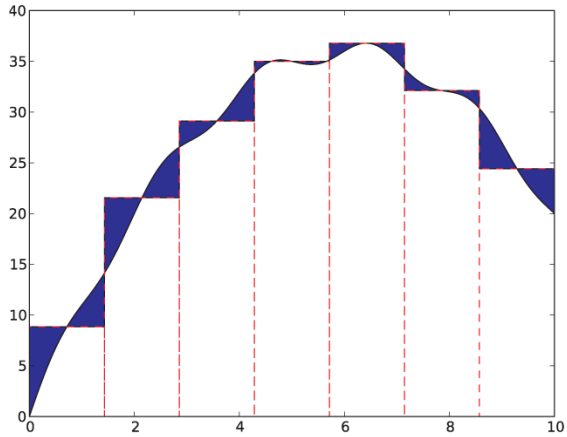
Hint. Obviously, the Trapezoidal method integrates linear functions exactly for any n. Another more surprising result is that the method is also exact for, e.g., $\int_0^{2\pi} \cos x \, dx$ for any n.
Filename: `trapezint.py`.

Remarks. Formula (3.10) is not the most common way of expressing the Trapezoidal integration rule. The reason is that $f(x_{i+1})$ is evaluated twice, first in term i and then as $f(x_i)$ in term $i+1$. The formula can be further developed to avoid unnecessary evaluations of $f(x_{i+1})$, which results in the standard form

$$\int_a^b f(x)dx \approx \frac{1}{2}h(f(a) + f(b)) + h\sum_{i=1}^{n-1} f(x_i)\,. \tag{3.11}$$

Exercise 3.7: Derive the general Midpoint integration rule

The idea of the Midpoint rule for integration is to divide the area under the curve $f(x)$ into n equal-sized rectangles (instead of trapezoids as in Exercise 3.6). The height of the rectangle is determined by the value of f at the midpoint of the rectangle. The figure below illustrates the idea.



Compute the area of each rectangle, sum them up, and arrive at the formula for the Midpoint rule:

$$\int_a^b f(x)dx \approx h\sum_{i=0}^{n-1} f(a+ih+\frac{1}{2}h), \tag{3.12}$$

where $h = (b-a)/n$ is the width of each rectangle. Implement this formula in a Python function `midpointint(f, a, b, n)` and test the function on the examples listed in Exercise 3.6b. How do the errors in the Midpoint rule compare with those of the Trapezoidal rule for $n = 1$ and $n = 10$? Filename: `midpointint.py`.

Exercise 3.8: Make an adaptive Trapezoidal rule

A problem with the Trapezoidal integration rule (3.10) in Exercise 3.6 is to decide how many trapezoids (n) to use in order to achieve a desired accuracy. Let E be the error in the Trapezoidal method, i.e., the difference between the exact integral and that produced by (3.10). We would like to prescribe a (small) tolerance ϵ and find an n such that $E \leq \epsilon$.

Since the exact value $\int_a^b f(x)dx$ is not available (that is why we use a numerical method!), it is challenging to compute E. Nevertheless, it has been shown by mathematicians that

$$E \leq \frac{1}{12}(b-a)h^2 \max_{x\in[a,b]} |f''(x)| \ . \tag{3.13}$$

The maximum of $|f''(x)|$ can be computed (approximately) by evaluating $f''(x)$ at a large number of points in $[a, b]$, taking the absolute value

$|f''(x)|$, and finding the maximum value of these. The double derivative can be computed by a finite difference formula:

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

With the computed estimate of $\max|f''(x)|$ we can find h from setting the right-hand side in (3.13) equal to the desired tolerance:

$$\frac{1}{12}(b-a)h^2 \max_{x\in[a,b]}|f''(x)| = \epsilon\,.$$

Solving with respect to h gives

$$h = \sqrt{12\epsilon}\left((b-a)\max_{x\in[a,b]}|f''(x)|\right)^{-1/2}\,. \tag{3.14}$$

With $n = (b-a)/h$ we have the n that corresponds to the desired accuracy ϵ.

a) Make a Python function `adaptive_trapezint(f, a, b, eps=1E-5)` for computing the integral $\int_a^b f(x)dx$ with an error less than or equal to ϵ (`eps`).

Hint. Compute the n corresponding to ϵ as explained above and call `trapezint(f, a, b, n)` from Exercise 3.6.

b) Apply the function to compute the integrals from Exercise 3.6b. Write out the exact error and the estimated n for each case.
Filename: `adaptive_trapezint.py`.

Remarks. A numerical method that applies an expression for the error to adapt the choice of the discretization parameter to a desired error tolerance, is known as an *adaptive* numerical method. The advantage of an adaptive method is that one can control the approximation error, and there is no need for the user to determine an appropriate number of intervals n.

Exercise 3.9: Explain why a program works

Explain how and thereby why the following program works:

```
def add(A, B):
    C = A + B
    return C

A = 3
B = 2
print add(A, B)
```

Exercise 3.10: Simulate a program by hand

Simulate the following program by hand to explain what is printed.

```
def a(x):
    q = 2
    x = 3*x
    return q + x

def b(x):
    global q
    q += x
    return q + x

q = 0
x = 3
print a(x), b(x), a(x), b(x)
```

Hint. If you encounter problems with understanding function calls and local versus global variables, paste the code into the Online Python Tutor[8] and step through the code to get a good explanation of what happens.

Exercise 3.11: Compute the area of an arbitrary triangle

An arbitrary triangle can be described by the coordinates of its three vertices: (x_1, y_1), (x_2, y_2), (x_3, y_3), numbered in a counterclockwise direction. The area of the triangle is given by the formula

$$A = \frac{1}{2}\left|x_2y_3 - x_3y_2 - x_1y_3 + x_3y_1 + x_1y_2 - x_2y_1\right| . \tag{3.15}$$

Write a function `area(vertices)` that returns the area of a triangle whose vertices are specified by the argument `vertices`, which is a nested list of the vertex coordinates. For example, computing the area of the triangle with vertex coordinates $(0, 0)$, $(1, 0)$, and $(0, 2)$ is done by

```
triangle1 = area([[0,0], [1,0], [0,2]])
# or
v1 = (0,0);  v2 = (1,0);  v3 = (0,2)
vertices = [v1, v2, v3]
triangle1 = area(vertices)

print 'Area of triangle is %.2f' % triangle1
```

Test the `area` function on a triangle with known area. Filename: `area_triangle.py`.

[8] `http://www.pythontutor.com/visualize.html`

Exercise 3.12: Compute the length of a path

Some object is moving along a path in the plane. At $n+1$ points of time we have recorded the corresponding (x, y) positions of the object: (x_0, y_0), (x_1, y_2), ..., (x_n, y_n). The total length L of the path from (x_0, y_0) to (x_n, y_n) is the sum of all the individual line segments ((x_{i-1}, y_{i-1}) to (x_i, y_i), $i = 1, \ldots, n$):

$$L = \sum_{i=1}^{n} \sqrt{(x_i - x_{i-1})^2 + (y_i - y_{i-1})^2}\,. \tag{3.16}$$

a) Make a Python function `pathlength(x, y)` for computing L according to the formula. The arguments `x` and `y` hold all the $x_0, \ldots, x_n$ and $y_0, \ldots, y_n$ coordinates, respectively.

b) Write a test function `test_pathlength()` where you check that `pathlength` returns the correct length in a test problem.
Filename: `pathlength.py`.

Exercise 3.13: Approximate π

The value of π equals the circumference of a circle with radius $1/2$. Suppose we approximate the circumference by a polygon through $n+1$ points on the circle. The length of this polygon can be found using the `pathlength` function from Exercise 3.12. Compute $n+1$ points (x_i, y_i) along a circle with radius $1/2$ according to the formulas

$$x_i = \frac{1}{2}\cos(2\pi i/n), \quad y_i = \frac{1}{2}\sin(2\pi i/n), \quad i = 0, \ldots, n\,.$$

Call the `pathlength` function and write out the error in the approximation of π for $n = 2^k$, $k = 2, 3, \ldots, 10$. Filename: `pi_approx.py`.

Exercise 3.14: 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.py`.

Exercise 3.15: Approximate a function by a sum of sines

We consider the piecewise constant function

$$f(t) = \begin{cases} 1, & 0 < t < T/2, \\ 0, & t = T/2, \\ -1, & T/2 < t < T \end{cases} \tag{3.17}$$

Sketch this function on a piece of paper. One can approximate $f(t)$ by the sum

$$S(t; n) = \frac{4}{\pi} \sum_{i=1}^{n} \frac{1}{2i-1} \sin\left(\frac{2(2i-1)\pi t}{T}\right). \tag{3.18}$$

It can be shown that $S(t; n) \to f(t)$ as $n \to \infty$.

a) Write a Python function `S(t, n, T)` for returning the value of $S(t; n)$.

b) Write a Python function `f(t, T)` for computing $f(t)$.

c) Write out tabular information showing how the error $f(t) - S(t; n)$ varies with n and t for the cases where $n = 1, 3, 5, 10, 30, 100$ and $t = \alpha T$, with $T = 2\pi$, and $\alpha = 0.01, 0.25, 0.49$. Use the table to comment on how the quality of the approximation depends on α and n.
Filename: `sinesum1.py`.

Remarks. A sum of sine and/or cosine functions, as in (3.18), is called a *Fourier series*. Approximating a function by a Fourier series is a very important technique in science and technology. Exercise 5.39 asks for visualization of how well $S(t; n)$ approximates $f(t)$ for some values of n.

Exercise 3.16: Implement a Gaussian function

Make a Python function `gauss(x, m=0, s=1)` for computing the Gaussian function

$$f(x) = \frac{1}{\sqrt{2\pi}\, s} \exp\left[-\frac{1}{2}\left(\frac{x-m}{s}\right)^2\right].$$

Write out a nicely formatted table of x and $f(x)$ values for n uniformly spaced x values in $[m - 5s, m + 5s]$. (Choose m, s, and n as you like.)
Filename: `gaussian2.py`.

Exercise 3.17: 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)`. 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 a soft and hard boiled egg, of a small ($M = 47$ g) and large ($M = 67$ g) size, taken from the fridge ($T_o = 4$ C) and from a hot room ($T_o = 25$ C). Filename: `egg_func.py`.

Exercise 3.18: Write a function for numerical differentiation

The formula

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h} \tag{3.19}$$

can be used to find an approximate derivative of a mathematical function $f(x)$ if h is small.

a) Write a function `diff(f, x, h=1E-5)` that returns the approximation (3.19) of the derivative of a mathematical function represented by a Python function `f(x)`.

b) Write a function `test_diff()` that verifies the implementation of the function `diff`. As test case, one can use the fact that (3.19) is exact for quadratic functions. Follow the conventions of the pytest and nose testing frameworks, as outlined in Exercise 3.2 and Sections 3.3.3, 3.4.2, and H.6.

c) Apply (3.19) to differentiate

- $f(x) = e^x$ at $x = 0$,
- $f(x) = e^{-2x^2}$ at $x = 0$,
- $f(x) = \cos x$ at $x = 2\pi$,
- $f(x) = \ln x$ at $x = 1$.

Use $h = 0.01$. In each case, write out the error, i.e., the difference between the exact derivative and the result of (3.19). Collect these four examples in a function `application()`.
Filename: `centered_diff.py`.

Exercise 3.19: Implement the factorial function

The factorial of n is written as $n!$ and defined as

$$n! = n(n-1)(n-2)\cdots 2 \cdot 1, \tag{3.20}$$

with the special cases

$$1! = 1, \quad 0! = 1\,. \tag{3.21}$$

For example, $4! = 4{\cdot}3{\cdot}2{\cdot}1 = 24$, and $2! = 2{\cdot}1 = 2$. Write a Python function `fact(n)` that returns $n!$. (Do not simply call the ready-made function `math.factorial(n)` - that is considered cheating in this context!)

Hint. Return 1 immediately if x is 1 or 0, otherwise use a loop to compute $n!$.
Filename: `fact.py`.

Exercise 3.20: Compute velocity and acceleration from 1D position data

Suppose we have recorded GPS coordinates $x_0, \ldots, x_n$ at times $t_0, \ldots, t_n$ while running or driving along a straight road. We want to compute the velocity v_i and acceleration a_i from these position coordinates. Using finite difference approximations, one can establish the formulas

$$v_i \approx \frac{x_{i+1} - x_{i-1}}{t_{i+1} - t_{i-1})}, \tag{3.22}$$

$$a_i \approx 2(t_{i+1} - t_{i-1})^{-1} \left(\frac{x_{i+1} - x_i}{t_{i+1} - t_i} - \frac{x_i - x_{i-1}}{t_i - t_{i-1}} \right), \tag{3.23}$$

for $i = 1, \ldots, n-1$.

a) Write a Python function `kinematics(x, i, dt=1E-6)` for computing v_i and a_i, given the array `x` of position coordinates $x_0, \ldots, x_n$.

b) Write a Python function `test_kinematics()` for testing the implementation in the case of constant velocity V. Set $t_0 = 0$, $t_1 = 0.5$, $t_2 = 1.5$, and $t_3 = 2.2$, and $x_i = Vt_i$.
Filename: `kinematics1.py`.

Exercise 3.21: Find the max and min values of a function

The maximum and minimum values of a mathematical function $f(x)$ on $[a, b]$ can be found by computing f at a large number (n) of points and selecting the maximum and minimum values at these points. Write a Python function `maxmin(f, a, b, n=1000)` that returns the maximum and minimum value of a function `f(x)`. Also write a test function for verifying the implementation for $f(x) = \cos x$, $x \in [-\pi/2, 2\pi]$.

Hint. The x points where the mathematical function is to be evaluated can be uniformly distributed: $x_i = a + ih$, $i = 0, \ldots, n-1$, $h = (b-a)/(n-1)$. The Python functions `max(y)` and `min(y)` return the maximum and minimum values in the list `y`, respectively.
Filename: `maxmin_f.py`.

Exercise 3.22: 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.py`.

Exercise 3.23: Implement the Heaviside function

The following *step function* is known as the *Heaviside function* and is widely used in mathematics:

$$H(x) = \begin{cases} 0, & x < 0 \\ 1, & x \geq 0 \end{cases} \tag{3.24}$$

a) Implement $H(x)$ in a Python function `H(x)`.

b) Make a Python function `test_H()` for testing the implementation of `H(x)`. Compute $H(-10)$, $H(-10^{-15})$, $H(0)$, $H(10^{-15})$, $H(10)$ and test that the answers are correct.
Filename: `Heaviside.py`.

Exercise 3.24: Implement a smoothed Heaviside function

The Heaviside function (3.24) listed in Exercise 3.23 is discontinuous. It is in many numerical applications advantageous to work with a smooth version of the Heaviside function where the function itself and its first derivative are continuous. One such smoothed Heaviside function is

$$H_\epsilon(x) = \begin{cases} 0, & x < -\epsilon, \\ \frac{1}{2} + \frac{x}{2\epsilon} + \frac{1}{2\pi}\sin\left(\frac{\pi x}{\epsilon}\right), & -\epsilon \leq x \leq \epsilon \\ 1, & x > \epsilon \end{cases} \tag{3.25}$$

a) Implement $H_\epsilon(x)$ in a Python function `H_eps(x, eps=0.01)`.

b) Make a Python function `test_H_eps()` for testing the implementation of `H_eps`. Check the values of some $x < -\epsilon$, $x = -\epsilon$, $x = 0$, $x = \epsilon$, and some $x > \epsilon$.
Filename: `smoothed_Heaviside.py`.

Exercise 3.25: Implement an indicator function

In many applications there is need for an indicator function, which is 1 over some interval and 0 elsewhere. More precisely, we define

$$I(x; L, R) = \begin{cases} 1, & x \in [L, R], \\ 0, & \text{elsewhere} \end{cases} \tag{3.26}$$

a) Make two Python implementations of such an indicator function, one with a direct test if $x \in [L, R]$ and one that expresses the indicator function in terms of Heaviside functions (3.24):

$$I(x; L, R) = H(x - L)H(R - x)\,. \tag{3.27}$$

b) Make a test function for verifying the implementation of the functions in a). Check that correct values are returned for some $x < L$, $x = L$, $x = (L + R)/2$, $x = R$, and some $x > R$.
Filename: `indicator_func.py`.

Exercise 3.26: Implement a piecewise constant function

Piecewise constant functions have a lot of important applications when modeling physical phenomena by mathematics. A piecewise constant function can be defined as

$$f(x) = \begin{cases} v_0, & x \in [x_0, x_1), \\ v_1, & x \in [x_1, x_2), \\ \vdots & \\ v_i & x \in [x_i, x_{i+1}), \\ \vdots & \\ v_n & x \in [x_n, x_{n+1}] \end{cases} \tag{3.28}$$

That is, we have a union of non-overlapping intervals covering the domain $[x_0, x_{n+1}]$, and $f(x)$ is constant in each interval. One example is the function that is -1 on $[0, 1]$, 0 on $[1, 1.5]$, and 4 on $[1.5, 2]$, where we with the notation in (3.28) have $x_0 = 0, x_1 = 1, x_2 = 1.5, x_3 = 2$ and $v_0 = -1, v_1 = 0, v_3 = 4$.

a) Make a Python function `piecewise(x, data)` for evaluating a piecewise constant mathematical function as in (3.28) at the point `x`. The `data` object is a list of pairs (v_i, x_i) for $i = 0, \ldots, n$. For example, `data` is `[(0, -1), (1, 0), (1.5, 4)]` in the example listed above. Since x_{n+1} is not a part of the `data` object, we have no means for detecting whether `x` is to the right of the last interval $[x_n, x_{n+1}]$, i.e., we must assume that the user of the `piecewise` function sends in an $x \leq x_{n+1}$.

b) Design suitable test cases for the function `piecewise` and implement them in a test function `test_piecewise()`.
Filename: `piecewise_constant1.py`.

Exercise 3.27: Apply indicator functions

Implement piecewise constant functions, as defined in Exercise 3.26, by observing that

$$f(x) = \sum_{i=0}^{n} v_i I(x; x_i, x_{i+1}), \tag{3.29}$$

where $I(x; x_i, x_{i+1})$ is the indicator function from Exercise 3.25. Filename: `piecewise_constant2.py`.

Exercise 3.28: Test your understanding of branching

Consider the following code:

```
def where1(x, y):
    if x > 0:
        print 'quadrant I or IV'
    if y > 0:
        print 'quadrant I or II'

def where2(x, y):
    if x > 0:
        print 'quadrant I or IV'
    elif y > 0:
        print 'quadrant II'

for x, y in (-1, 1), (1, 1):
    where1(x,y)
    where2(x,y)
```

What is printed?

Exercise 3.29: Simulate nested loops by hand

Go through the code below by hand, statement by statement, and calculate the numbers that will be printed.

```
n = 3
for i in range(-1, n):
    if i != 0:
        print i

for i in range(1, 13, 2*n):
    for j in range(n):
        print i, j

for i in range(1, n+1):
    for j in range(i):
        if j:
            print i, j

for i in range(1, 13, 2*n):
    for j in range(0, i, 2):
        for k in range(2, j, 1):
            b = i > j > k
            if b:
                print i, j, k
```

You may use a debugger, see Section F.1, or the Online Python Tutor[9], see Section 3.1.2, to control what happens when you step through the code.

Exercise 3.30: Rewrite a mathematical function

We consider the $L(x;n)$ sum as defined in Section 3.1.8 and the corresponding function `L3(x, epsilon)` function from Section 3.1.10. The sum $L(x;n)$ can be written as

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

a) Derive a relation between c_i and c_{i-1},

$$c_i = ac_{i-1},$$

where a is an expression involving i and x.

b) The relation $c_i = ac_{i-1}$ means that we can start with `term` as c_1, and then in each pass of the loop implementing the sum $\sum_i c_i$ we can compute the next term c_i in the sum as

```
term = a*term
```

Write a new version of the `L3` function, called `L3_ci(x, epsilon)`, that makes use of this alternative computation of the terms in the sum.

c) Write a Python function `test_L3_ci()` that verifies the implementation of `L3_ci` by comparing with the original `L3` function.
Filename: `L3_recursive.py`.

Exercise 3.31: Make a table for approximations of $\cos x$

The function $\cos(x)$ can be approximated by the sum

$$C(x;n) = \sum_{j=0}^{n} c_j, \tag{3.30}$$

where

$$c_j = -c_{j-1}\frac{x^2}{2j(2j-1)}, \quad j = 1, 2, \ldots, n,$$

and $c_0 = 1$.

a) Make a Python function for computing $C(x;n)$.

[9] `http://www.pythontutor.com/`

Hint. Represent c_j by a variable `term`, make updates `term = -term*...` inside a `for` loop, and accumulate the `term` variable in a variable for the sum.

b) Make a function for writing out a table of the errors in the approximation $C(x;n)$ of $\cos(x)$ for some x and n values given as arguments to the function. Let the x values run downward in the rows and the n values to the right in the columns. For example, a table for $x = 4\pi, 6\pi, 8\pi, 10\pi$ and $n = 5, 25, 50, 100, 200$ can look like

```
      x          5          25          50         100         200
 12.5664   1.61e+04   1.87e-11   1.74e-12   1.74e-12   1.74e-12
 18.8496   1.22e+06   2.28e-02   7.12e-11   7.12e-11   7.12e-11
 25.1327   2.41e+07   6.58e+04  -4.87e-07  -4.87e-07  -4.87e-07
 31.4159   2.36e+08   6.52e+09   1.65e-04   1.65e-04   1.65e-04
```

Observe how the error increases with x and decreases with n.
Filename: `cos_sum.py`.

Exercise 3.32: Use None in keyword arguments

Consider the functions `L2(x, n)` and `L3(x, epsilon)` from Sections 3.1.8 and 3.1.10, whose program code is found in the file `lnsum.py`.

Make a more flexible function `L4` where we can either specify a tolerance `epsilon` *or* a number of terms `n` in the sum. Moreover, we can also choose whether we want the sum to be returned or the sum and the number of terms:

```
value, n = L4(x, epsilon=1E-8, return_n=True)
value = L4(x, n=100)
```

Hint. The starting point for all this flexibility is to have some keyword arguments initialized to an "undefined" value, called `None`, which can be recognized inside the function:

```
def L3(x, n=None, epsilon=None, return_n=False):
    if n is not None:
        ...
    if epsilon is not None:
        ...
```

One can also apply `if n != None`, but the `is` operator is most common.

Print error messages for incompatible values when `n` *and* `epsilon` are `None` or both are given by the user.
Filename: `L4.py`.

Exercise 3.33: Write a sort function for a list of 4-tuples

Below is a list of the nearest stars and some of their properties. The list elements are 4-tuples containing the name of the star, the distance from

the sun in light years, the apparent brightness, and the luminosity. The apparent brightness is how bright the stars look in our sky compared to the brightness of Sirius A. The luminosity, or the true brightness, is how bright the stars would look if all were at the same distance compared to the Sun. The list data are found in the file `stars.txt`[10], which looks as follows:

```
data = [
('Alpha Centauri A',    4.3,  0.26,      1.56),
('Alpha Centauri B',    4.3,  0.077,     0.45),
('Alpha Centauri C',    4.2,  0.00001,   0.00006),
("Barnard's Star",      6.0,  0.00004,   0.0005),
('Wolf 359',            7.7,  0.000001,  0.00002),
('BD +36 degrees 2147', 8.2,  0.0003,    0.006),
('Luyten 726-8 A',      8.4,  0.000003,  0.00006),
('Luyten 726-8 B',      8.4,  0.000002,  0.00004),
('Sirius A',            8.6,  1.00,      23.6),
('Sirius B',            8.6,  0.001,     0.003),
('Ross 154',            9.4,  0.00002,   0.0005),
]
```

The purpose of this exercise is to sort this list with respect to distance, apparent brightness, and luminosity. Write a program that initializes the `data` list as above and writes out three sorted tables: star name versus distance, star name versus apparent brightness, and star name versus luminosity.

Hint. To sort a list `data`, one can call `sorted(data)`, as in

```
for item in sorted(data):
    ...
```

However, in the present case each element is a 4-tuple, and the default sorting of such 4-tuples results in a list with the stars appearing in alphabetic order. This is not what you want. Instead, we need to sort with respect to the 2nd, 3rd, or 4th element of each 4-tuple. If such a tailored sort mechanism is necessary, we can provide our own sort function as a second argument to `sorted`: `sorted(data, mysort)`. A sort function `mysort` must take two arguments, say `a` and `b`, and return -1 if `a` should become before `b` in the sorted sequence, 1 if `b` should become before `a`, and 0 if they are equal. In the present case, `a` and `b` are 4-tuples, so we need to make the comparison between the right elements in `a` and `b`. For example, to sort with respect to luminosity we can write

```
def mysort(a, b):
    if a[3] < b[3]:
        return -1
    elif a[3] > b[3]:
        return 1
    else:
        return 0
```

Filename: `sorted_stars_data.py`.

[10] `http://tinyurl.com/pwyasaa/funcif/stars.txt`

Exercise 3.34: Find prime numbers

The *Sieve of Eratosthenes* is an algorithm for finding all prime numbers less than or equal to a number N. Read about this algorithm on Wikipedia and implement it in a Python program. Filename: `find_primes.py`.

Exercise 3.35: Find pairs of characters

Write a function `count_pairs(dna, pair)` that returns the number of occurrences of a pair of characters (`pair`) in a DNA string (`dna`). For example, calling the function with `dna` as `'ACTGCTATCCATT'` and `pair` as `'AT'` will return 2. Filename: `count_pairs.py`.

Exercise 3.36: Count substrings

This is an extension of Exercise 3.35: count how many times a certain string appears in another string. For example, the function returns 3 when called with the DNA string `'ACGTTACGGAACG'` and the substring `'ACG'`.

Hint. For each match of the first character of the substring in the main string, check if the next `n` characters in the main string matches the substring, where `n` is the length of the substring. Use slices like `s[3:9]` to pick out a substring of `s`.
Filename: `count_substr.py`.

Exercise 3.37: Resolve a problem with a function

Consider the following interactive session:

```
>>> def f(x):
...     if 0 <= x <= 2:
...         return x**2
...     elif 2 < x <= 4:
...         return 4
...     elif x < 0:
...         return 0
...
>>> f(2)
4
>>> f(5)
>>> f(10)
```

Why do we not get any output when calling `f(5)` and `f(10)`?

Hint. Save the `f` value in a variable `r` and do `print r`.

Exercise 3.38: Determine the types of some objects

Consider the following calls to the `makelist` function from Section 3.1.6:

```
l1 = makelist(0, 100, 1)
l2 = makelist(0, 100, 1.0)
l3 = makelist(-1, 1, 0.1)
l4 = makelist(10, 20, 20)
l5 = makelist([1,2], [3,4], [5])
l6 = makelist((1,-1,1), ('myfile.dat', 'yourfile.dat'))
l7 = makelist('myfile.dat', 'yourfile.dat', 'herfile.dat')
```

Simulate each call by hand to determine what type of objects that become elements in the returned list and what the contents of `value` is after one pass in the loop.

Hint. Note that some of the calls will lead to infinite loops if you really perform the above `makelist` calls on a computer.

You can go to the Online Python Tutor[11], paste in the `makelist` function and the session above, and step through the program to see what actually happens.

Remarks. This exercise demonstrates that we can write a function and have in mind certain types of arguments, here typically `int` and `float` objects. However, the function can be used with other (originally unintended) arguments, such as lists and strings in the present case, leading to strange and irrelevant behavior (the problem here lies in the boolean expression `value <= stop` which is meaningless for some of the arguments).

Exercise 3.39: Find an error in a program

Consider the following program for computing

$$f(x) = e^{rx}\sin(mx) + e^{sx}\sin(nx)\,.$$

```
def f(x, m, n, r, s):
    return expsin(x, r, m) + expsin(x, s, n)

x = 2.5
print f(x, 0.1, 0.2, 1, 1)

from math import exp, sin

def expsin(x, p, q):
    return exp(p*x)*sin(q*x)
```

Running this code results in

```
NameError: global name 'expsin' is not defined
```

What is the problem? Simulate the program flow by hand, use the debugger to step from line to line, or use the Online Python Tutor. Correct the program.

[11] http://www.pythontutor.com/