Array Computing and Curve Plotting

5

A list object is handy for storing tabular data, such as a sequence of objects or a table of objects. An array is very similar to a list, but less flexible and computationally much more efficient. When using the computer to perform mathematical calculations, we often end up with a huge amount of numbers and associated arithmetic operations. Storing numbers in lists may in such contexts lead to slow programs, while arrays can make the programs run much faster. This is crucial for many advanced applications of mathematics in industry and science, where computer programs may run for hours and days, or even weeks. Any clever idea that reduces the execution time by some factor is therefore paramount.

However, one can argue that programmers of mathematical software have traditionally paid too much attention to efficiency and "clever" program constructs. The resulting software often becomes very hard to maintain and extend. In this book we advocate a focus on clear, well-designed, and easy-to-understand programs that work correctly. Thereafter, one can start thinking about optimization for speed. Fortunately, arrays contribute to clear code, correctness and speed – all at once.

This chapter gives an introduction to arrays: how they are created and what they can be used for. Array computing usually ends up with a lot of numbers. It may be very hard to understand what these numbers mean by just looking at them. Since the human is a visual animal, a good way to understand numbers is to visualize them. In this chapter we concentrate on visualizing curves that reflect functions of one variable; i.e., curves of the form $y = f(x)$. A synonym for curve is graph, and the image of curves on the screen is often called a plot. We will use arrays to store the information about points along the curve. In a nutshell, array computing demands visualization and visualization demands arrays.

All program examples in this chapter can be found as files in the folder `src/plot`[1].

[1] http://tinyurl.com/pwyasaa/plot

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5.1 Vectors

This section gives a brief introduction to the vector concept, assuming that you have heard about vectors in the plane and maybe vectors in space before. This background will be valuable when we start to work with arrays and curve plotting.

5.1.1 The Vector Concept

Some mathematical quantities are associated with a set of numbers. One example is a point in the plane, where we need two coordinates (real numbers) to describe the point mathematically. Naming the two coordinates of a particular point as x and y, it is common to use the notation (x, y) for the point. That is, we group the numbers inside parentheses. Instead of symbols we might use the numbers directly: $(0, 0)$ and $(1.5, -2.35)$ are also examples of coordinates in the plane.

A point in three-dimensional space has three coordinates, which we may name x_1, x_2, and x_3. The common notation groups the numbers inside parentheses: (x_1, x_2, x_3). Alternatively, we may use the symbols x, y, and z, and write the point as (x, y, z), or numbers can be used instead of symbols.

From high school you may have a memory of solving two equations with two unknowns. At the university you will soon meet problems that are formulated as n equations with n unknowns. The solution of such problems contains n numbers that we can collect inside parentheses and number from 1 to n: $(x_1, x_2, x_3, \ldots, x_{n-1}, x_n)$.

Quantities such as (x, y), (x, y, z), or $(x_1, \ldots, x_n)$ are known as *vectors* in mathematics. A visual representation of a vector is an arrow that goes from the origin to a point. For example, the vector (x, y) is an arrow that goes from $(0, 0)$ to the point with coordinates (x, y) in the plane. Similarly, (x, y, z) is an arrow from $(0, 0, 0)$ to the point (x, y, z) in three-dimensional space.

Mathematicians found it convenient to introduce spaces with higher dimension than three, because when we have a solution of n equations collected in a vector $(x_1, \ldots, x_n)$, we may think of this vector as a point in a space with dimension n, or equivalently, an arrow that goes from the origin $(0, \ldots, 0)$ in n-dimensional space to the point $(x_1, \ldots, x_n)$. Figure 5.1 illustrates a vector as an arrow, either starting at the origin, or at any other point. Two arrows/vectors that have the same direction and the same length are mathematically equivalent.

We say that $(x_1, \ldots, x_n)$ is an n-vector or a vector with n components. Each of the numbers x_1, x_2, ... is a component or an element. We refer to the first component (or element), the second component (or element), and so forth.

A Python program may use a list or tuple to represent a vector:

```
v1 = [x, y]          # list of variables
v2 = (-1, 2)         # tuple of numbers
v3 = (x1, x2, x3)    # tuple of variables
from math import exp
v4 = [exp(-i*0.1) for i in range(150)]
```

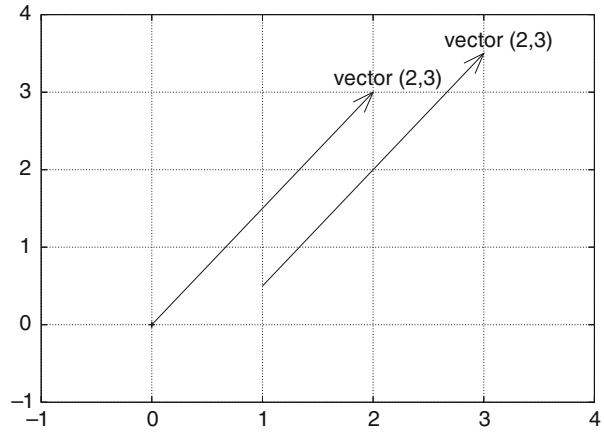


Fig. 5.1 A vector $(2, 3)$ visualized in the standard way as an arrow from the origin to the point $(2, 3)$, and mathematically equivalently, as an arrow from $(1, \frac{1}{2})$ (or any point (a, b)) to $(3, 3\frac{1}{2})$ (or $(a + 2, b + 3)$)

While `v1` and `v2` are vectors in the plane and `v3` is a vector in three-dimensional space, `v4` is a vector in a 150-dimensional space, consisting of 150 values of the exponential function. Since Python lists and tuples have 0 as the first index, we may also in mathematics write the vector (x_1, x_2) as (x_0, x_1). This is not at all common in mathematics, but makes the distance from a mathematical description of a problem to its solution in Python shorter.

It is impossible to visually demonstrate how a space with 150 dimensions looks like. Going from the plane to three-dimensional space gives a rough feeling of what it means to add a dimension, but if we forget about the idea of a visual perception of space, the mathematics is very simple: going from a 4-dimensional vector to a 5-dimensional vector is just as easy as adding an element to a list of symbols or numbers.

5.1.2 Mathematical Operations on Vectors

Since vectors can be viewed as arrows having a length and a direction, vectors are extremely useful in geometry and physics. The velocity of a car has a magnitude and a direction, so has the acceleration, and the position of a point in the car is also a vector. An edge of a triangle can be viewed as a line (arrow) with a direction and length.

In geometric and physical applications of vectors, mathematical operations on vectors are important. We shall exemplify some of the most important operations on vectors below. The goal is not to teach computations with vectors, but more to illustrate that such computations are defined by mathematical rules. Given two vectors, (u_1, u_2) and (v_1, v_2), we can add these vectors according to the rule:

$$(u_1, u_2) + (v_1, v_2) = (u_1 + v_1, u_2 + v_2)\,. \tag{5.1}$$

We can also subtract two vectors using a similar rule:

$$(u_1, u_2) - (v_1, v_2) = (u_1 - v_1, u_2 - v_2)\,. \tag{5.2}$$

A vector can be multiplied by a number. This number, called a below, is usually denoted as a *scalar*:

$$a \cdot (v_1, v_2) = (av_1, av_2)\,. \tag{5.3}$$

The inner product, also called dot product, or scalar product, of two vectors is a number:

$$(u_1, u_2) \cdot (v_1, v_2) = u_1 v_1 + u_2 v_2\,. \tag{5.4}$$

(From high school mathematics and physics you might recall that the inner or dot product also can be expressed as the product of the lengths of the two vectors multiplied by the cosine of the angle between them, but we will not make use of that formula. There is also a *cross product* defined for 2-vectors or 3-vectors, but we do not list the cross product formula here.)

The length of a vector is defined by

$$||(v_1, v_2)|| = \sqrt{(v_1, v_2) \cdot (v_1, v_2)} = \sqrt{v_1^2 + v_2^2}\,. \tag{5.5}$$

The same mathematical operations apply to n-dimensional vectors as well. Instead of counting indices from 1, as we usually do in mathematics, we now count from 0, as in Python. The addition and subtraction of two vectors with n components (or elements) read

$$(u_0, \ldots, u_{n-1}) + (v_0, \ldots, v_{n-1}) = (u_0 + v_0, \ldots, u_{n-1} + v_{n-1}), \tag{5.6}$$

$$(u_0, \ldots, u_{n-1}) - (v_0, \ldots, v_{n-1}) = (u_0 - v_0, \ldots, u_{n-1} - v_{n-1})\,. \tag{5.7}$$

Multiplication of a scalar a and a vector $(v_0, \ldots, v_{n-1})$ equals

$$(av_0, \ldots, av_{n-1})\,. \tag{5.8}$$

The inner or dot product of two n-vectors is defined as

$$(u_0, \ldots, u_{n-1}) \cdot (v_0, \ldots, v_{n-1}) = u_0 v_0 + \cdots + u_{n-1} v_{n-1} = \sum_{j=0}^{n-1} u_j v_j\,. \tag{5.9}$$

Finally, the length $||v||$ of an n-vector $v = (v_0, \ldots, v_{n-1})$ is

$$\begin{aligned}\sqrt{(v_0, \ldots, v_{n-1}) \cdot (v_0, \ldots, v_{n-1})} &= \left(v_0^2 + v_1^2 + \cdots + v_{n-1}^2\right)^{\frac{1}{2}} \\ &= \left(\sum_{j=0}^{n-1} v_j^2\right)^{\frac{1}{2}}\,.\end{aligned} \tag{5.10}$$

5.1.3 Vector Arithmetics and Vector Functions

In addition to the operations on vectors in Sect. 5.1.2, which you might recall from high school mathematics, we can define other operations on vectors. This is very useful for speeding up programs. Unfortunately, the forthcoming vector operations are hardly treated in textbooks on mathematics, yet these operations play a significant role in mathematical software, especially in computing environment such as MATLAB, Octave, Python, and R.

Applying a mathematical function of one variable, $f(x)$, to a vector is defined as a vector where f is applied to each element. Let $v = (v_0, \ldots, v_{n-1})$ be a vector. Then

$$f(v) = (f(v_0), \ldots, f(v_{n-1})) .$$

For example, the sine of v is

$$\sin(v) = (\sin(v_0), \ldots, \sin(v_{n-1})) .$$

It follows that squaring a vector, or the more general operation of raising the vector to a power, can be defined as applying the operation to each element:

$$v^b = (v_0^b, \ldots, v_{n-1}^b) .$$

Another operation between two vectors that arises in computer programming of mathematics is the "asterisk" multiplication, defined as

$$u * v = (u_0 v_0, u_1 v_1, \ldots, u_{n-1} v_{n-1}) . \tag{5.11}$$

Adding a scalar to a vector or array can be defined as adding the scalar to each component. If a is a scalar and v a vector, we have

$$a + v = (a + v_0, \ldots, a + v_{n-1}) .$$

A compound vector expression may look like

$$v^2 * \cos(v) * e^v + 2 . \tag{5.12}$$

How do we calculate this expression? We use the normal rules of mathematics, working our way, term by term, from left to right, paying attention to the fact that powers are evaluated before multiplications and divisions, which are evaluated prior to addition and subtraction. First we calculate v^2, which results in a vector we may call u. Then we calculate $\cos(v)$ and call the result p. Then we multiply $u * p$ to get a vector which we may call w. The next step is to evaluate e^v, call the result q, followed by the multiplication $w * q$, whose result is stored as r. Then we add $r + 2$ to get the final result. It might be more convenient to list these operations after each other:

- $u = v^2$
- $p = \cos(v)$
- $w = u * p$

- $q = e^v$
- $r = w * q$
- $s = r + 2$

Writing out the vectors u, w, p, q, and r in terms of a general vector $v = (v_0, \ldots, v_{n-1})$ (do it!) shows that the result of the expression (5.12) is the vector

$$(v_0^2 \cos(v_0)e^{v_0} + 2, \ldots, v_{n-1}^2 \cos(v_{n-1})e^{v_{n-1}} + 2) .$$

That is, component no. i in the result vector equals the number arising from applying the formula (5.12) to v_i, where the * multiplication is ordinary multiplication between two numbers.

We can, alternatively, introduce the function

$$f(x) = x^2 \cos(x)e^x + 2$$

and use the result that $f(v)$ means applying f to each element in v. The result is the same as in the vector expression (5.12).

In Python programming it is important for speed (and convenience too) that we can apply functions of one variable, like $f(x)$, to vectors. What this means mathematically is something we have tried to explain in this subsection. Doing Exercises 5.5 and 5.6 may help to grasp the ideas of vector computing, and with more programming experience you will hopefully discover that vector computing is very useful. It is not necessary to have a thorough understanding of vector computing in order to proceed with the next sections.

Arrays are used to represent vectors in a program, but one can do more with arrays than with vectors. Until Sect. 5.8 it suffices to think of arrays as the same as vectors in a program.

5.2 Arrays in Python Programs

This section introduces array programming in Python, but first we create some lists and show how arrays differ from lists.

5.2.1 Using Lists for Collecting Function Data

Suppose we have a function $f(x)$ and want to evaluate this function at a number of x points $x_0, x_1, \ldots, x_{n-1}$. We could collect the n pairs $(x_i, f(x_i))$ in a list, or we could collect all the x_i values, for $i = 0, \ldots, n-1$, in a list and all the associated $f(x_i)$ values in another list. The following interactive session demonstrates how to create these three types of lists:

```
>>> def f(x):
...     return x**3       # sample function
...
```

```
>>> n = 5                  # no of points along the x axis
>>> dx = 1.0/(n-1)         # spacing between x points in [0,1]
>>> xlist = [i*dx for i in range(n)]
>>> ylist = [f(x) for x in xlist]
>>> pairs = [[x, y] for x, y in zip(xlist, ylist)]
```

Here we have used list comprehensions for achieving compact code. Make sure that you understand what is going on in these list comprehensions (if not, try to write the same code using standard `for` loops and appending new list elements in each pass of the loops).

The list elements consist of objects of the same type: any element in `pairs` is a list of two `float` objects, while any element in `xlist` or `ylist` is a `float`. Lists are more flexible than that, because an element can be an object of any type, e.g.,

```
mylist = [2, 6.0, 'tmp.pdf', [0,1]]
```

Here `mylist` holds an `int`, a `float`, a string, and a list. This combination of diverse object types makes up what is known as *heterogeneous* lists. We can also easily remove elements from a list or add new elements anywhere in the list. This flexibility of lists is in general convenient to have as a programmer, but in cases where the elements are of the same type and the number of elements is fixed, arrays can be used instead. The benefits of arrays are faster computations, less memory demands, and extensive support for mathematical operations on the data. Because of greater efficiency and mathematical convenience, arrays will be used to a large extent in this book. The great use of arrays is also prominent in other programming environments such as MATLAB, Octave, and R, for instance. Lists will be our choice instead of arrays when we need the flexibility of adding or removing elements or when the elements may be of different object types.

5.2.2 Basics of Numerical Python Arrays

An *array* object can be viewed as a variant of a list, but with the following assumptions and features:

- All elements must be of the same type, preferably integer, real, or complex numbers, for efficient numerical computing and storage.
- The number of elements must be known when the array is created.
- Arrays are not part of standard Python – one needs an additional package called *Numerical Python*, often abbreviated as NumPy. The Python name of the package, to be used in `import` statements, is `numpy`.
- With `numpy`, a wide range of mathematical operations can be done directly on complete arrays, thereby removing the need for loops over array elements. This is commonly called *vectorization*
- Arrays with one index are often called vectors. Arrays with two indices are used as an efficient data structure for tables, instead of lists of lists. Arrays can also have three or more indices.

We have two remarks to the above list. First, there is actually an object type called `array` in standard Python, but this data type is not so efficient for mathematical computations, and we will not use it in this book. Second, the number of elements in an array *can* be changed, but at a substantial computational cost.

The following text lists some important functionality of NumPy arrays. A more comprehensive treatment is found in the excellent *NumPy Tutorial*, *NumPy User Guide*, *NumPy Reference*, *Guide to NumPy*, and *NumPy for MATLAB Users*, all accessible at scipy.org[2].

The standard import statement for Numerical Python reads

```
import numpy as np
```

To convert a list `r` to an array, we use the `array` function from `numpy`:

```
a = np.array(r)
```

To create a new array of length `n`, filled with zeros, we write

```
a = np.zeros(n)
```

The array elements are of a type that corresponds to Python's `float` type. A second argument to `np.zeros` can be used to specify other element types, e.g., `int`. A similar function,

```
a = np.zeros_like(c)
```

generates an array of zeros where the length is that of the array `c` and the element type is the same as those in `c`. Arrays with more than one index are treated in Sect. 5.8.

Often one wants an array to have n elements with uniformly distributed values in an interval $[p, q]$. The `numpy` function `linspace` creates such arrays:

```
a = np.linspace(p, q, n)
```

Array elements are accessed by square brackets as for lists: `a[i]`. Slices also work as for lists, for example, `a[1:-1]` picks out all elements except the first and the last, but contrary to lists, `a[1:-1]` is not a copy of the data in `a`. Hence,

```
b = a[1:-1]
b[2] = 0.1
```

will also change `a[3]` to `0.1`. A slice `a[i:j:s]` picks out the elements starting with index `i` and stepping `s` indices at the time up to, but not including, `j`. Omitting `i` implies `i=0`, and omitting `j` implies `j=n` if `n` is the number of elements in the array. For example, `a[0:-1:2]` picks out every two elements up to, but not including, the last element, while `a[::4]` picks out every four elements in the whole array.

[2] http://scipy.org

Remarks on importing NumPy

The statement

```
import numpy as np
```

with subsequent prefixing of all NumPy functions and variables by `np`, has evolved as a standard syntax in the Python scientific computing community. However, to make Python programs look closer to MATLAB and ease the transition to and from that language, one can do

```
from numpy import *
```

to get rid of the prefix (this is evolved as the standard in *interactive* Python shells). This author prefers mathematical functions from `numpy` to be written without the prefix to make the formulas as close as possible to the mathematics. So, $f(x) = \sinh(x-1)\sin(wt)$ would be coded as

```
from numpy import sinh, sin

def f(x):
    return sinh(x-1)*sin(w*t)
```

or one may take the less recommended lazy approach `from numpy import *` and fill up the program with *a lot* of functions and variables from `numpy`.

5.2.3 Computing Coordinates and Function Values

With these basic operations at hand, we can continue the session from the previous section and make arrays out of the lists `xlist` and `ylist`:

```
>>> import numpy as np
>>> x2 = np.array(xlist)      # turn list xlist into array x2
>>> y2 = np.array(ylist)
>>> x2
array([ 0.  ,  0.25,  0.5 ,  0.75,  1.  ])
>>> y2
array([ 0.      ,  0.015625,  0.125   ,  0.421875,  1.      ])
```

Instead of first making a list and then converting the list to an array, we can compute the arrays directly. The equally spaced coordinates in `x2` are naturally computed by the `np.linspace` function. The `y2` array can be created by `np.zeros`, to ensure that `y2` has the right length `len(x2)`, and then we can run a `for` loop to fill in all elements in `y2` with `f` values:

```
>>> n = len(xlist)
>>> x2 = np.linspace(0, 1, n)
>>> y2 = np.zeros(n)
```

```
>>> for i in xrange(n):
...     y2[i] = f(x2[i])
...
>>> y2
array([ 0.      ,  0.015625,  0.125   ,  0.421875,  1.      ])
```

Note that we here in the `for` loop have used `xrange` instead of `range`. The former is faster for long loops because it avoids generating *and storing* a list of integers, it just generates the values one by one. Hence, we prefer `xrange` over `range` for loops over long arrays. In Python version 3.x, `range` is the same as `xrange`.

Creating an array of a given length is frequently referred to as *allocating* the array. It simply means that a part of the computer's memory is marked for being occupied by this array. Mathematical computations will often fill up most of the computer's memory by allocating long arrays.

We can shorten the previous code by creating the `y2` data in a list comprehension, but list comprehensions produce lists, not arrays, so we need to transform the list object to an array object:

```
>>> x2 = np.linspace(0, 1, n)
>>> y2 = np.array([f(xi) for xi in x2])
```

Nevertheless, there is a much faster way of computing `y2` as the next paragraph explains.

5.2.4 Vectorization

Loops over very long arrays may run slowly. A great advantage with arrays is that we can get rid of the loops and apply `f` directly to the whole array:

```
>>> y2 = f(x2)
>>> y2
array([ 0.      ,  0.015625,  0.125   ,  0.421875,  1.      ])
```

The magic that makes `f(x2)` work builds on the vector computing concepts from Sect. 5.1.3. Instead of calling `f(x2)` we can equivalently write the function formula `x2**3` directly.

The point is that `numpy` implements vector arithmetics *for arrays* of any dimension. Moreover, `numpy` provides its own versions of mathematical functions like `cos`, `sin`, `exp`, `log`, etc., which work for array arguments and apply the mathematical function to each element. The following code, computes each array element separately:

```
from math import sin, cos, exp
import numpy as np
x = np.linspace(0, 2, 201)
r = np.zeros(len(x))
for i in xrange(len(x)):
    r[i] = sin(np.pi*x[i])*cos(x[i])*exp(-x[i]**2) + 2 + x[i]**2
```

while here is a corresponding code that operates on arrays directly:

```
r = np.sin(np.pi*x)*np.cos(x)*np.exp(-x**2) + 2 + x**2
```

Many will prefer to see such formulas without the `np` prefix:

```
from numpy import sin, cos, exp, pi
r = sin(pi*x)*cos(x)*exp(-x**2) + 2 + x**2
```

An important thing to understand is that `sin` from the `math` module is different from the `sin` function provided by `numpy`. The former does not allow array arguments, while the latter accepts both real numbers and arrays.

Replacing a loop like the one above, for computing `r[i]`, by a vector/array expression like `sin(x)*cos(x)*exp(-x**2) + 2 + x**2`, is called *vectorization*. The loop version is often referred to as *scalar code*. For example,

```
import numpy as np
import math
x = np.zeros(N);  y = np.zeros(N)
dx = 2.0/(N-1) # spacing of x coordinates
for i in range(N):
    x[i] = -1 + dx*i
    y[i] = math.exp(-x[i])*x[i]
```

is scalar code, while the corresponding vectorized version reads

```
x = np.linspace(-1, 1, N)
y = np.exp(-x)*x
```

We remark that list comprehensions,

```
x = array([-1 + dx*i for i in range(N)])
y = array([np.exp(-xi)*xi for xi in x])
```

result in scalar code because we still have explicit, slow Python `for` loops operating on scalar quantities. The requirement of vectorized code is that there are no explicit Python `for` loops. The loops required to compute each array element are performed in fast C or Fortran code in the `numpy` package.

Most Python functions intended for a scalar argument `x`, like

```
def f(x):
    return x**4*exp(-x)
```

automatically work for an array argument `x`:

```
x = np.linspace(-3, 3, 101)
y = f(x)
```

provided that the `exp` function in the definition of `f` accepts an array argument. This means that `exp` must have been imported as `from numpy import *` or explicitly as `from numpy import exp`. One can, of course, prefix `exp` as in `np.exp`, at the loss of a less attractive mathematical syntax in the formula.

When a Python function `f(x)` works for an array argument `x`, we say that the function `f` is vectorized. Provided that the mathematical expressions in `f` involve arithmetic operations and basic mathematical functions from the `math` module, `f` will be automatically vectorized by just importing the functions from `numpy` instead of `math`. However, if the expressions inside `f` involve `if` tests, the code needs a rewrite to work with arrays. Section 5.4.1 presents examples where we have to do special actions in order to vectorize functions.

Vectorization is very important for speeding up Python programs that perform heavy computations with arrays. Moreover, vectorization gives more compact code that is easier to read. Vectorization is particularly important for statistical simulations, as demonstrated in Chap. 8.

5.3 Curve Plotting

Visualizing a function $f(x)$ is done by drawing the curve $y = f(x)$ in an xy coordinate system. When we use a computer to do this task, we say that we *plot* the curve. Technically, we plot a curve by drawing straight lines between n points on the curve. The more points we use, the smoother the curve appears.

Suppose we want to plot the function $f(x)$ for $a \leq x \leq b$. First we pick out n x coordinates in the interval $[a, b]$, say we name these $x_0, x_1, \ldots, x_{n-1}$. Then we evaluate $y_i = f(x_i)$ for $i = 0, 1, \ldots, n-1$. The points (x_i, y_i), $i = 0, 1, \ldots, n-1$, now lie on the curve $y = f(x)$. Normally, we choose the x_i coordinates to be equally spaced, i.e.,

$$x_i = a + ih, \quad h = \frac{b-a}{n-1}.$$

If we store the x_i and y_i values in two arrays `x` and `y`, we can plot the curve by a command like `plot(x,y)`.

Sometimes the names of the independent variable and the function differ from x and f, but the plotting procedure is the same. Our first example of curve plotting demonstrates this fact by involving a function of t.

5.3.1 MATLAB-Style Plotting with Matplotlib

The standard package for curve plotting in Python is Matplotlib. We first exemplify a usage of this package that is very similar with how you plot in MATLAB as many readers will have MATLAB knowledge of will need to operate MATLAB at some point.

A basic plot Let us plot the curve $y = t^2 \exp(-t^2)$ for t values between 0 and 3. First we generate equally spaced coordinates for t, say 51 values (50 intervals). Then we compute the corresponding y values at these points, before we call the `plot(t,y)` command to make the curve plot. Here is the complete program:

```
from numpy import *
from matplotlib.pyplot import *

def f(t):
    return t**2*exp(-t**2)

t = linspace(0, 3, 51)    # 51 points between 0 and 3
y = zeros(len(t))         # allocate y with float elements
for i in xrange(len(t)):
    y[i] = f(t[i])

plot(t, y)
show()
```

In this program we pre-allocate the y array and fill it with values, element by element, in a Python loop. Alternatively, we may operate on the whole `t` array at once, which yields faster and shorter code:

```
y = f(t)
```

To include the plot in electronic documents, we need a hardcopy of the figure in PDF, PNG, or another image format. The `savefig` function saves the plot to files in various image formats:

```
savefig('tmp1.pdf') # produce PDF
savefig('tmp1.png') # produce PNG
```

The filename extension determines the format: `.pdf` for PDF and `.png` for PNG. Figure 5.2 displays the resulting plot.

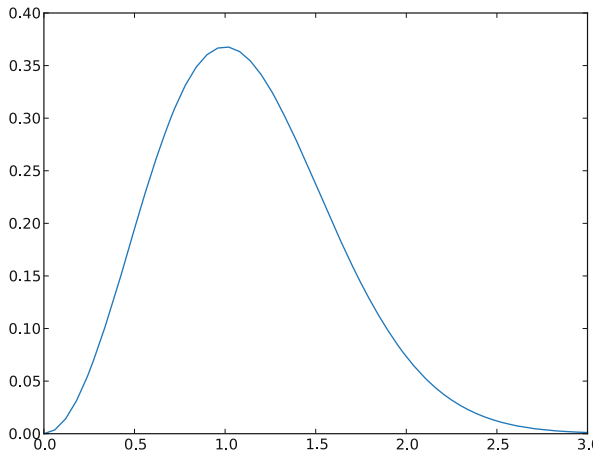


Fig. 5.2 A simple plot in PDF format (Matplotlib)

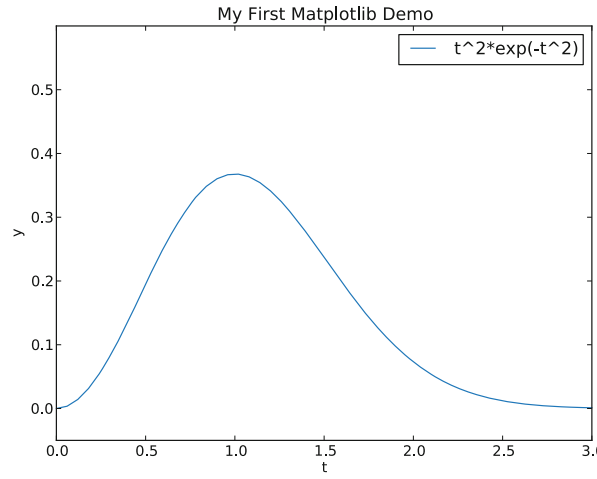


Fig. 5.3 A single curve with label, title, and axis adjusted (Matplotlib)

Decorating the plot The x and y axes in curve plots should have labels, here t and y, respectively. Also, the curve should be identified with a label, or legend as it is often called. A title above the plot is also common. In addition, we may want to control the extent of the axes (although most plotting programs will automatically adjust the axes to the range of the data). All such things are easily added after the `plot` command:

```
plot(t, y)
xlabel('t')
ylabel('y')
legend(['t^2*exp(-t^2)'])
axis([0, 3, -0.05, 0.6])   # [tmin, tmax, ymin, ymax]
title('My First Matplotlib Demo')
savefig('tmp2.pdf')
show()
```

Removing the `show()` call prevents the plot from being shown on the screen, which is advantageous if the program's purpose is to make a large number of plots in PDF or PNG format (you do not want all the plot windows to appear on the screen and then kill all of them manually). This decorated plot is displayed in Fig. 5.3.

Plotting multiple curves A common plotting task is to compare two or more curves, which requires multiple curves to be drawn in the same plot. Suppose we want to plot the two functions $f_1(t) = t^2 \exp(-t^2)$ and $f_2(t) = t^4 \exp(-t^2)$. We can then just issue two `plot` commands, one for each function. To make the syntax resemble MATLAB, we call `hold('on')` after the first `plot` command to indicate that subsequent `plot` commands are to draw the curves in the first plot.

```
def f1(t):
    return t**2*exp(-t**2)
```

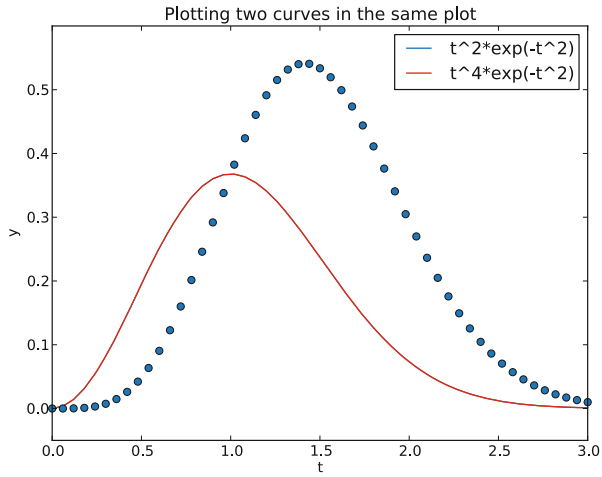


Fig. 5.4 Two curves in the same plot (Matplotlib)

```
def f2(t):
    return t**2*f1(t)

t = linspace(0, 3, 51)
y1 = f1(t)
y2 = f2(t)

plot(t, y1, 'r-')
hold('on')
plot(t, y2, 'bo')
xlabel('t')
ylabel('y')
legend(['t^2*exp(-t^2)', 't^4*exp(-t^2)'])
title('Plotting two curves in the same plot')
show()
```

In these `plot` commands, we have also specified the line type: `r-` means red (`r`) line (`-`), while `bo` means a blue (`b`) circle (`o`) at each data point. Figure 5.4 shows the result. The legends for each curve is specified in a list where the sequence of strings correspond to the sequence of `plot` commands. Doing a `hold('off')` makes the next `plot` command create a new plot.

Placing several plots in one figure We may also put plots together in a figure with `r` rows and `c` columns of plots. The `subplot(r,c,a)` does this, where `a` is a row-wise counter for the individual plots. Here is an example with two rows of plots, and one plot in each row, (see Fig. 5.5):

```
figure()  # make separate figure
subplot(2, 1, 1)
t = linspace(0, 3, 51)
y1 = f1(t)
y2 = f2(t)
```

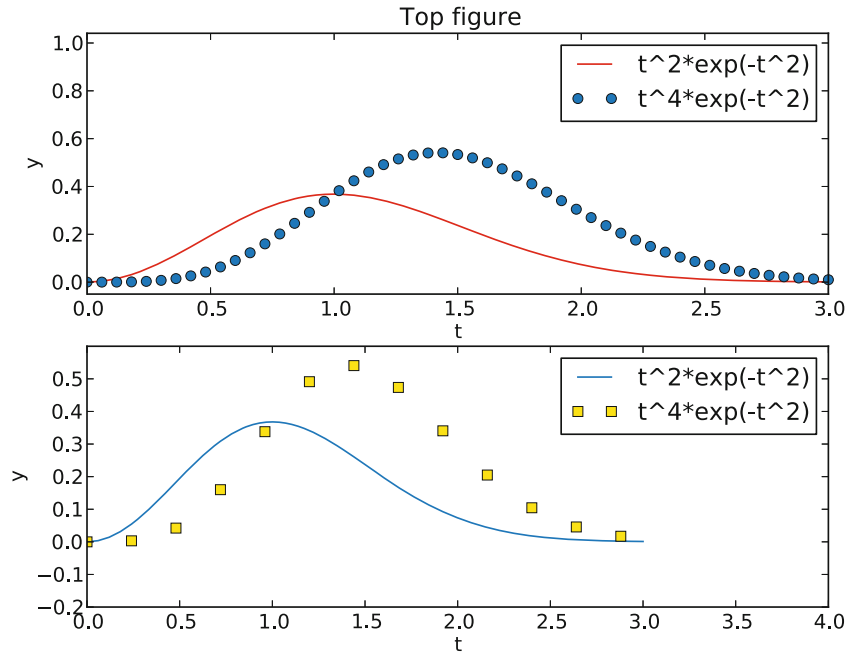


Fig. 5.5 Example on two plots in one figure (Matplotlib)

```
plot(t, y1, 'r-', t, y2, 'bo')
xlabel('t')
ylabel('y')
axis([t[0], t[-1], min(y2)-0.05, max(y2)+0.5])
legend(['t^2*exp(-t^2)', 't^4*exp(-t^2)'])
title('Top figure')

subplot(2, 1, 2)
t3 = t[::4]
y3 = f2(t3)

plot(t, y1, 'b-', t3, y3, 'ys')
xlabel('t')
ylabel('y')
axis([0, 4, -0.2, 0.6])
legend(['t^2*exp(-t^2)', 't^4*exp(-t^2)'])
savefig('tmp4.pdf')
show()
```

The `figure()` call creates a new plot window on the screen.

All of the examples above on plotting with Matplotlib are collected in the file `mpl_pylab_examples.py`.

5.3.2 Matplotlib; Pyplot Prefix

The Matplotlib developers do not promote the plotting style we exemplified above. Instead, they recommend to prefix plotting commands by the `matplotlib.pyplot` module and also prefix array computing commands to demonstrate that they come from Numerical Python:

```
import numpy as np
import matplotlib.pyplot as plt
```

The plot in Fig. 5.3 can typically be obtained by prefixing the previously shown plotting commands with `plt`:

```
plt.plot(t, y)
plt.legend(['t^2*exp(-t^2)'])
plt.xlabel('t')
plt.ylabel('y')
plt.axis([0, 3, -0.05, 0.6])   # [tmin, tmax, ymin, ymax]
plt.title('My First Matplotlib Demo')
plt.show()
plt.savefig('tmp2.pdf') # produce PDF
```

Instead of giving plot data and legends separately, it is more common to write

```
plt.plot(t, y, label='t^2*exp(-t^2)')
```

However, in this book we shall stick to the `legend` command since this makes the transition to/from MATLAB easier.

Figure 5.4 can be produced by

```
def f1(t):
    return t**2*np.exp(-t**2)

def f2(t):
    return t**2*f1(t)

t = np.linspace(0, 3, 51)
y1 = f1(t)
y2 = f2(t)

plt.plot(t, y1, 'r-')
plt.plot(t, y2, 'bo')
plt.xlabel('t')
plt.ylabel('y')
plt.legend(['t^2*exp(-t^2)', 't^4*exp(-t^2)'])
plt.title('Plotting two curves in the same plot')
plt.savefig('tmp3.pdf')
plt.show()
```

Putting multiple plots in a figure follows the same set-up with `subplot` as previously shown, except that commands are prefixed by `plt`. The complete example, along with the codes listed above, are found in the file `mpl_pyplot_examples.py`.

Once you have created a basic plot, there are numerous possibilities for fine-tuning the figure, i.e., adjusting tick marks on the axis, inserting text, etc. The Matplotlib website is full of instructive examples on what you can do with this excellent package.

5.3.3 SciTools and Easyviz

Matplotlib has become the *de facto* standard for curve plotting in Python, but there are several other alternative packages, especially if we also consider plotting of 2D/3D scalar and vector fields. Python has interfaces to many leading visualization packages: MATLAB, Gnuplot, Grace, OpenDX, and VTK. Even basic plotting with these packages has very different syntax, and deciding what package and syntax to go with was and still is a challenge. As a response to this challenge, Easyviz was created to provide a common uniform interface to all the mentioned visualization packages (including Matplotlib). The syntax of this interface was made very close to that of MATLAB, since most scientists and engineers have experience with MATLAB or most probably will be using it in some context. (In general, the Python syntax used in the examples in this book is constructed to ease the transition to and from MATLAB.)

Easyviz is part of the SciTools package, which consists of a set of Python tools building on Numerical Python, ScientificPython, the comprehensive SciPy environment, and other packages for scientific computing with Python. SciTools contains in particular software related to the book [13] and the present text. Installation is straightforward as described on the web page https://github.com/hplgit/scitools.

Importing SciTools and Easyviz A standard import of SciTools is

```
from scitools.std import *
```

The advantage of this statement is that it, with a minimum of typing, imports a lot of useful modules for numerical Python programming: Easyviz for MATLAB-style plotting, all of `numpy` (`from numpy import *`), all of `scipy` (`from scipy import *`) if available, the `StringFunction` tool (see Sect. 4.3.3), many mathematical functions and tools in SciTools, plus commonly applied modules such as `sys`, `os`, and `math`. The imported standard mathematical functions (`sqrt`, `sin`, `asin`, `exp`, etc.) are from `numpy.lib.scimath` and deal transparently with real and complex input/output (as the corresponding MATLAB functions):

```
>>> from scitools.std import *
>>> a = array([-4., 4])
>>> sqrt(a)                 # need complex output
array([ 0.+2.j,  2.+0.j])
>>> a = array([16., 4])
>>> sqrt(a)                 # can reduce to real output
array([ 4.,  2.])
```

The inverse trigonometric functions have different names in `math` and `numpy`, a fact that prevents an expression written for scalars, using `math` names, to be

immediately valid for arrays. Therefore, the `from scitools.std import *` action also imports the names `asin`, `acos`, and `atan` for the `numpy` or `scipy` names `arcsin`, `arccos`, and `arctan` functions, to ease vectorization of mathematical expressions involving inverse trigonometric functions.

The downside of the "star import" from `scitools.std` is twofold. First, it fills up your program or interactive session with the names of several hundred functions. Second, when using a particular function, you do not know the package it comes from. Both problems are solved by doing an import of the type used in Sect. 5.3.2:

```
import scitools.std as st
import numpy as np
```

All of the SciTools and Easyviz functions must then be prefixed by `st`. Although the `numpy` functions are available through the `st` prefix, we recommend using the `np` prefix to clearly see where functionality comes from.

Since the Easyviz syntax for plotting is very close to that of MATLAB, it is also very close to the syntax of Matplotlib shown earlier. This will be demonstrated in the forthcoming examples. The advantage of using Easyviz is that the underlying plotting package, used to create the graphics and known as a *backend*, can trivially be replaced by another package. If users of your Python software have not installed a particular visualization package, the software can still be used with another alternative (which might be considerably easier to install). By default, Easyviz now employs Matplotlib for plotting. Other popular alternatives are Gnuplot and MATLAB. For 2D/3D scalar and vector fields, VTK is a popular backend for Easyviz.

We shall next redo the curve plotting examples from Sect. 5.3.1 using Easyviz syntax.

A basic plot Plotting the curve $y = t^2 \exp(-t^2)$ for $t \in [0, 3]$, using 31 equally spaced points (30 intervals) is performed by like this:

```
from scitools.std import *

def f(t):
    return t**2*exp(-t**2)

t = linspace(0, 3, 31)
y = f(t)
plot(t, y, '-')
```

To save the plot in a file, we use the `savefig` function, which takes the filename as argument:

```
savefig('tmp1.pdf') # produce PDF
savefig('tmp1.eps') # produce PostScript
savefig('tmp1.png') # produce PNG
```

The filename extension determines the format: `.pdf` for PDF, `.ps` or `.eps` for PostScript, and `.png` for PNG. A synonym for the `savefig` function is `hardcopy`.

What if the plot window quickly disappears?
On some platforms, some backends may result in a plot that is shown in just a fraction of a second on the screen before the plot window disappears (the Gnuplot backend on Windows machines and the Matplotlib backend constitute two examples). To make the window stay on the screen, add

```
raw_input('Press the Return key to quit: ')
```

at the end of the program. The plot window is killed when the program terminates, and this statement postpones the termination until the user hits the Return key.

Decorating the plot Let us plot the same curve, but now with a legend, a plot title, labels on the axes, and specified ranges of the axes:

```
from scitools.std import *

def f(t):
    return t**2*exp(-t**2)

t = linspace(0, 3, 31)
y = f(t)
plot(t, y, '-')
xlabel('t')
ylabel('y')
legend('t^2*exp(-t^2)')
axis([0, 3, -0.05, 0.6])   # [tmin, tmax, ymin, ymax]
title('My First Easyviz Demo')
```

Easyviz has also introduced a more Pythonic `plot` command where all the plot properties can be set at once through keyword arguments:

```
plot(t, y, '-',
     xlabel='t',
     ylabel='y',
     legend='t^2*exp(-t^2)',
     axis=[0, 3, -0.05, 0.6],
     title='My First Easyviz Demo',
     savefig='tmp1.pdf',
     show=True)
```

With `show=False` one can avoid the plot window on the screen and just make the plot file.

Note that we in the curve legend write `t` square as `t^2` (LaTeX style) rather than `t**2` (program style). Whichever form you choose is up to you, but the LaTeX form sometimes looks better in some plotting programs (Matplotlib and Gnuplot are two examples).

Plotting multiple curves Next we want to compare the two functions $f_1(t) = t^2 \exp(-t^2)$ and $f_2(t) = t^4 \exp(-t^2)$. Writing two `plot` commands after each other

makes two separate plots. To make the second curve appear together with the first one, we need to issue a `hold('on')` call after the first `plot` command. All subsequent `plot` commands will then draw curves in the same plot, until `hold('off')` is called.

```
from scitools.std import *

def f1(t):
    return t**2*exp(-t**2)

def f2(t):
    return t**2*f1(t)

t = linspace(0, 3, 51)
y1 = f1(t)
y2 = f2(t)

plot(t, y1, 'r-')
hold('on')
plot(t, y2, 'b-')

xlabel('t')
ylabel('y')
legend('t^2*exp(-t^2)', 't^4*exp(-t^2)')
title('Plotting two curves in the same plot')
savefig('tmp3.pdf')
```

The sequence of the multiple legends is such that the first legend corresponds to the first curve, the second legend to the second curve, and so forth.

Instead of separate calls to `plot` and the use of `hold('on')`, we can do everything at once and just send several curves to `plot`:

```
plot(t, y1, 'r-', t, y2, 'b-', xlabel='t', ylabel='y',
     legend=('t^2*exp(-t^2)', 't^4*exp(-t^2)'),
     title='Plotting two curves in the same plot',
     savefig='tmp3.pdf')
```

Throughout this book, we very often make use of this type of compact `plot` command, which also only requires an import of the form `from scitools.std import plot`.

Changing backend Easyviz applies Matplotlib for plotting by default, so the resulting figures so far will be similar to those of Fig. 5.2–5.4.

However, we can use other backends (plotting packages) for creating the graphics. The specification of what package to use is defined in a configuration file (see the heading *Setting Parameters in the Configuration File* in the Easyviz documentation), or on the command line:

Terminal

```
Terminal> python myprog.py --SCITOOLS_easyviz_backend gnuplot
```

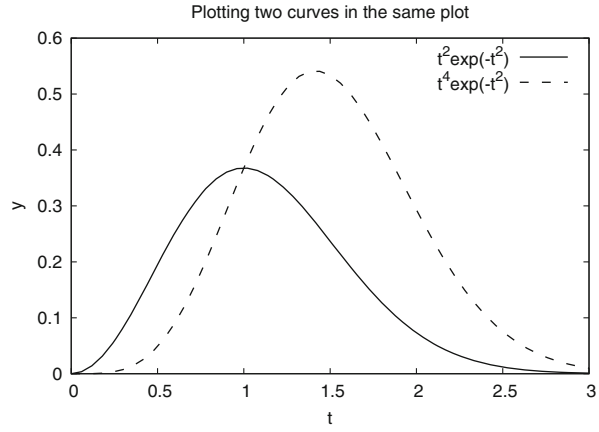


Fig. 5.6 Two curves in the same plot (Gnuplot)

Now, the plotting commands in `myprog.py` will make use of Gnuplot to create the graphics, with a slightly different result than that created by Matplotlib (compare Figs. 5.4 and 5.6). A nice feature of Gnuplot is that the line types are automatically changed if we save a figure to file, such that the lines are easily distinguishable in a black-and-white plot. With Matplotlib one has to carefully set the line types to make them effective on a grayscale.

Placing several plots in one figure Finally, we redo the example from Sect. 5.3.1 where two plots are combined into one figure, using the `subplot` command:

```
figure()
subplot(2, 1, 1)
t = linspace(0, 3, 51)
y1 = f1(t)
y2 = f2(t)
plot(t, y1, 'r-', t, y2, 'bo', xlabel='t', ylabel='y',
     legend=('t^2*exp(-t^2)', 't^4*exp(-t^2)'),
     axis=[t[0], t[-1], min(y2)-0.05, max(y2)+0.5],
     title='Top figure')

subplot(2, 1, 2)
t3 = t[::4]
y3 = f2(t3)

plot(t, y1, 'b-', t3, y3, 'ys',
     xlabel='t', ylabel='y',
     axis=[0, 4, -0.2, 0.6],
     legend=('t^2*exp(-t^2)', 't^4*exp(-t^2)'))
savefig('tmp4.pdf')
```

Note that `figure()` must be used if you want a program to make different plot windows on the screen: each `figure()` call creates a new, separate plot.

All of the Easyviz examples above are found in the file `easyviz_examples.py`. We remark that Easyviz is just a thin layer of code providing access to the most

common plotting functionality for curves as well as 2D/3D scalar and vector fields. Fine-tuning of plots, e.g., specifying tick marks on the axes, is not supported, simply because most of the curve plots in the daily work can be made without such functionality. For fine-tuning the plot with special commands, you need to grab an object in Easyviz that communicates directly with the underlying plotting package used to create the graphics. With this object you can issue package-specific commands and do whatever the underlying package allows you do. This is explained in the Easyviz manual[3], which also comes up by running `pydoc scitools.easyviz`. As soon as you have digested the very basics of plotting, you are strongly recommend to read through the curve plotting part of the Easyviz manual.

5.3.4 Making Animations

A sequence of plots can be combined into an animation on the screen and stored in a video file. The standard procedure is to generate a series of individual plots and to show them in sequence to obtain an animation effect. Plots store in files can be combined to a video file.

Example The function

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

is known as the Gaussian function or the probability density function of the normal (or Gaussian) distribution. This bell-shaped function is wide for large s and peak-formed for small s, see Fig. 5.7. The function is symmetric around $x = m$ ($m = 0$ in the figure). Our goal is to make an animation where we see how this function evolves as s is decreased. In Python we implement the formula above as a function `f(x, m, s)`.

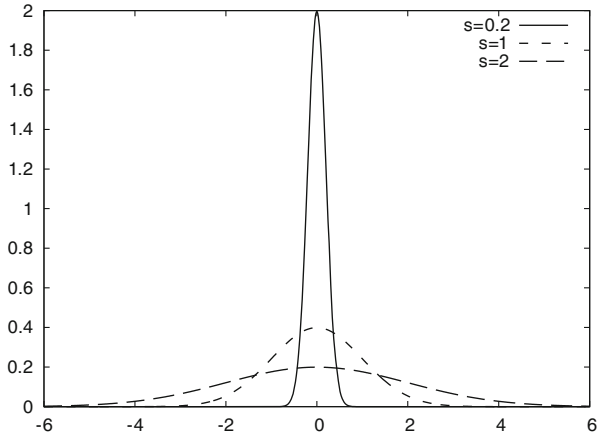


Fig. 5.7 Different shapes of a Gaussian function

[3] https://scitools.googlecode.com/hg/doc/easyviz/easyviz.html

The animation is created by varying s in a loop and for each s issue a `plot` command. A moving curve is then visible on the screen. One can also make a video that can be played as any other computer movie using a standard movie player. To this end, each plot is saved to a file, and all the files are combined together using some suitable tool to be explained later. Before going into programming detail there is one key point to emphasize.

Keep the extent of axes fixed during animations!

The underlying plotting program will normally adjust the axis to the maximum and minimum values of the curve if we do not specify the axis ranges explicitly. For an animation such automatic axis adjustment is misleading – any axis range must be fixed to avoid a jumping axis.

The relevant values for the y axis range in the present example is the minimum and maximum value of f. The minimum value is zero, while the maximum value appears for $x = m$ and increases with decreasing s. The range of the y axis must therefore be $[0, f(m; m, \min s)]$.

The function f is defined for all $-\infty < x < \infty$, but the function value is very small already $3s$ away from $x = m$. We may therefore limit the x coordinates to $[m - 3s, m + 3s]$.

Animation in Easyviz We start with using Easyviz for animation since this is almost identical to making standard static plots, and you can choose the plotting engine you want to use, say Gunplot or Matplotlib. The Easyviz recipe for animating the Gaussian function as s goes from 2 to 0.2 looks as follows.

```
from scitools.std import sqrt, pi, exp, linspace, plot, movie
import time

def f(x, m, s):
    return (1.0/(sqrt(2*pi)*s))*exp(-0.5*((x-m)/s)**2)

m = 0
s_min = 0.2
s_max = 2
x = linspace(m -3*s_max, m + 3*s_max, 1000)
s_values = linspace(s_max, s_min, 30)
# f is max for x=m; smaller s gives larger max value
max_f = f(m, m, s_min)

# Show the movie on the screen
# and make hardcopies of frames simultaneously.

counter = 0
for s in s_values:
    y = f(x, m, s)
    plot(x, y, '-', axis=[x[0], x[-1], -0.1, max_f],
         xlabel='x', ylabel='f', legend='s=%4.2f' % s,
         savefig='tmp%04d.png' % counter)
    counter += 1
    #time.sleep(0.2)  # can insert a pause to control movie speed
```

Note that the s values are decreasing (`linspace` handles this automatically if the start value is greater than the stop value). Also note that we, simply because we think it is visually more attractive, let the y axis go from -0.1 although the f function is always greater than zero. The complete code is found in the file `movie1.py`.

Notice

It is crucial to use the single, compound `plot` command shown above, where axis, labels, legends, etc., are set in the same call. Splitting up in individual calls to `plot`, `axis`, and so forth, results in jumping curves and axis. Also, when visualizing more than one animated curve at a time, make sure you send all data to a single `plot` command.

Remark on naming plot files

For each frame (plot) in the movie we store the plot in a file, with the purpose of combining all the files to an ordinary video file. The different files need different names such that various methods for listing the files will list them in the correct order. To this end, we recommend using filenames of the form `tmp0001.png`, `tmp0002.png`, `tmp0003.png`, etc. The printf format `04d` pads the integers with zeros such that `1` becomes `0001`, `13` becomes `0013` and so on. The expression `tmp*.png` will now expand (by an alphabetic sort) to a list of all files in proper order.

Without the padding with zeros, i.e., names of the form `tmp1.png`, `tmp2.png`, ..., `tmp12.png`, etc., the alphabetic order will give a wrong sequence of frames in the movie. For instance, `tmp12.png` will appear before `tmp2.png`.

Basic animation in Matplotlib Animation is Matplotib requires more than a loop over a parameter and making a plot inside the loop. The set-up that is closest to standard static plots is shown first, while the newer and more widely used tool `FuncAnimation` is explained afterwards.

The first part of the program, where we define `f`, `x`, `s_values`, and so forth, is the same regardless of the animation technique. Therefore, we concentrate on the graphics part here:

```
import matplotlib.pyplot as plt
...
# Make a first plot
plt.ion()
y = f(x, m, s_max)
lines = plt.plot(x, y)
plt.axis([x[0], x[-1], -0.1, max_f])
plt.xlabel('x')
plt.ylabel('f')

# Show the movie, and make hardcopies of frames simulatenously
counter = 0
for s in s_values:
    y = f(x, m, s)
    lines[0].set_ydata(y)
```

```
    plt.legend(['s=%4.2f' % s])
    plt.draw()
    plt.savefig('tmp_%04d.png' % counter)
    counter += 1
```

The `plt.ion()` call is important, so is the first plot, where we grab the result of the `plot` command, which is a list of Matplotlib's `Line2D` objects. The idea is then to update the data via `lines[0].set_ydata` and show the plot via `plt.draw()` for each frame. For multiple curves we must update the y data for each curve, e.g.,

```
lines = plot(x, y1, x, y2, x, y3)

for parameter in parameters:
    y1 = ...
    y2 = ...
    y3 = ...
    for line, y in zip(lines, [y1, y2, y3]):
        line.set_ydata(y)
    plt.draw()
```

The file movie1_mpl1.py contains the complete program for doing animation with native Matplotlib syntax.

Using FuncAnimation in Matplotlib The recommended approach to animation in Matplotlib is to use the `FuncAnimation` tool:

```
import matplotlib.pyplot as plt
from matplotlib.animation import animation

anim = animation.FuncAnimation(
    fig, frame, all_args, interval=150, init_func=init, blit=True)
```

Here, `fig` is the `plt.figure()` object for the current figure, `frame` is a user-defined function for plotting each frame, `all_args` is a list of arguments for `frame`, `interval` is the delay in ms between each frame, `init_func` is a function called for defining the background plot in the animation, and `blit=True` speeds up the animation. For frame number `i`, `FuncAnimation` will call `frame(all_args[i])`. Hence, the user's task is mostly to write the `frame` function and construct the `all_args` arguments.

After having defined `m`, `s_max`, `s_min`, `s_values`, and `max_f` as shown earlier, we have to make a first plot:

```
fig = plt.figure()
plt.axis([x[0], x[-1], -0.1, max_f])
lines = plt.plot([], [])
plt.xlabel('x')
plt.ylabel('f')
```

Notice that we save the return value of `plt.plot` in `lines` such that we can conveniently update the data for the curve(s) in each frame.

The function for defining a background plot draws an empty plot in this example:

```
def init():
    lines[0].set_data([], [])  # empty plot
    return lines
```

The function that defines the individual plots in the animation basically computes y from f and updates the data of the curve:

```
def frame(args):
    frame_no, s, x, lines = args
    y = f(x, m, s)
    lines[0].set_data(x, y)
    return lines
```

Multiple curves can be updated as shown earlier.

We are now ready to call `animation.FuncAnimation`:

```
anim = animation.FuncAnimation(
    fig, frame, all_args, interval=150, init_func=init, blit=True)
```

A common next action is to make a video file, here in the MP4 format with 5 frames per second:

```
anim.save('movie1.mp4', fps=5)   # movie in MP4 format
```

Finally, we must `plt.show()` as always to watch any plots on the screen.

The video making requires additional software on the computer, such as `ffmpeg`, and can fail. One gets more control over the potentially fragile movie making process by explicitly saving plots to file and explicitly running movie making programs like `ffmeg` later. Such programs are explained in Sect. 5.3.5.

The complete code showing the basic use of `FuncAnimation` is available in `movie1_FuncAnimation.py`. There is also a MATLAB Animation Tutorial[4] with more basic information, plus a set of animation examples on http://matplotlib.org/examples.

Remove old plot files!

We strongly recommend removing previously generated plot files before a new set of files is made. Otherwise, the movie may get old and new files mixed up. The following Python code removes all files of the form `tmp*.png`:

```
import glob, os
for filename in glob.glob('tmp*.png'):
    os.remove(filename)
```

These code lines should be inserted at the beginning of programs or functions performing animations.

[4] http://jakevdp.github.io/blog/2012/08/18/matplotlib-animation-tutorial/

Instead of deleting the individual plotfiles, one may store all plot files in a subfolder and later delete the subfolder. Here is a suitable code segment:

```
import shutil, os
subdir = 'temp'            # subfolder name for plot files
if os.path.isdir(subdir):  # does the subfolder already exist?
    shutil.rmtree(subdir)  # delete the whole folder
os.mkdir(subdir)           # make new subfolder
os.chdir(subdir)           # move to subfolder
# ... perform all the plotting, make movie ...
os.chdir(os.pardir)        # optional: move up to parent folder
```

Note that Python and many other languages use the word directory instead of folder. Consequently, the name of functions dealing with folders have a name containing `dir` for directory.

5.3.5 Making Videos

Suppose we have a set of frames in an animation, saved as plot files `tmp_*.png`. The filenames are generated by the printf syntax `'tmp_%04d.png' % i`, using a frame counter `i` that goes from 0 to some value. The corresponding files are then `tmp_0000.png`, `tmp_0001.png`, `tmp_0002.png`, and so on. Several tools can be used to create videos in common formats from the individual frames in the plot files.

Animated GIF file The ImageMagick[5] software suite contains a program `convert` for making animated GIF files:

Terminal

```
Terminal> convert -delay 50 tmp_*.png movie.gif
```

The delay between frames, here 50, is measured in units of 1/100 s. The resulting animated GIF file `movie.gif` can be viewed by another program in the ImageMagick suite: `animate movie.gif`, but the most common way of displaying animated GIF files is to include them in web pages. Writing the HTML code

```
<img src="movie.gif">
```

in some file with extension `.html` and loading this file into a web browser will play the movie repeatedly. You may try this out online[6].

MP4, Ogg, WebM, and Flash videos The modern video formats that are best suited for being displayed in web browsers are MP4, Ogg, WebM, and Flash. The program `ffmpeg`, or the almost equivalent `avconv`, is a common tool to create such movies. Creating a flash video is done by

[5] http://www.imagemagick.org/
[6] http://hplgit.github.io/scipro-primer/video/gaussian.html

Terminal

```
Terminal> ffmpeg -i tmp_%04d.png -r 5 -vcodec flv movie.flv
```

The `-i` option specifies the printf string that was used to make the names of the individual plot files, `-r` specifies the number of frames per second, here 5, `-vcodec` is the video codec for Flash, which is called `flv`, and the final argument is the name of the video file. On Debian Linux systems, such as Ubuntu, you use the `avconv` program instead of `ffmpeg`.

Other formats are created in the same way, but we need to specify the codec and use the right extension in the video file:

Format	Codec and filename
Flash	`-vcodec flv movie.flv`
MP4	`-vcodec libx264 movie.mp4`
Webm	`-vcodec libvpx movie.webm`
Ogg	`-vcodec libtheora movie.ogg`

Video files are normally trivial to play in graphical file browser: double lick the filename or right-click and choose a player. On Linux systems there are several players that can be run from the command line, e.g., `vlc`, `mplayer`, `gxine`, and `totem`.

It is easy to create the video file from a Python program since we can run any operating system command in (e.g.) `os.system`:

```
cmd = 'convert -delay 50 tmp_*.png movie.gif'
os.system(cmd)
```

It might happen that your downloaded and installed version of `ffmpeg` fails to generate videos in some of the mentioned formats. The reason is that `ffmpeg` depends on many other packages that may be missing on your system. Getting `ffmpeg` to work with the `libx264` codec for making MP4 files is often challenging. On Debian-based Linux systems, such as Ubuntu, the installation procedure at the time of this writing goes like

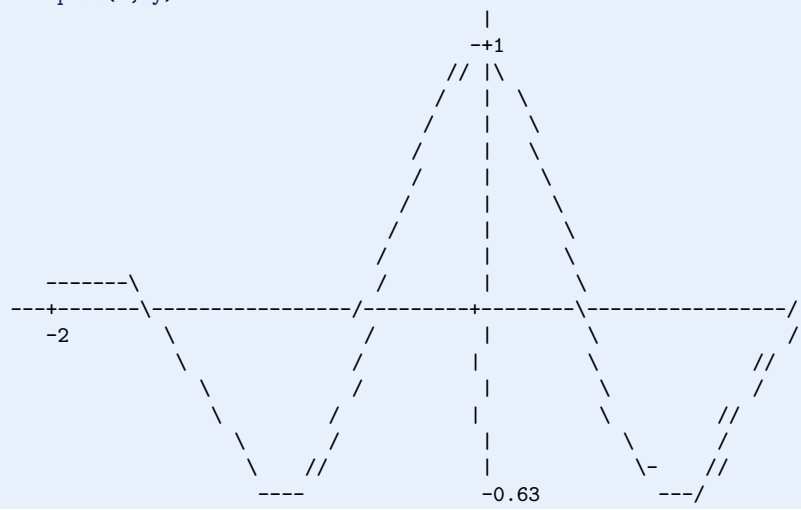
Terminal

```
Terminal> sudo apt-get install lib-avtools libavcodec-extra-53 \
          libx264-dev
```

5.3.6 Curve Plots in Pure Text

Sometimes it can be desirable to show a graph in pure ASCII text, e.g., as part of a trial run of a program included in the program itself, or a graph that can be illustrative in a doc string. For such purposes we have slightly extended a module by Imri Goldberg (`aplotter.py`) and included it as a module in SciTools. Running `pydoc` on `scitools.aplotter` describes the capabilities of this type of primitive plotting. Here we just give an example of what it can do:

```
>>> import numpy as np
>>> x = np.linspace(-2, 2, 81)
>>> y = np.exp(-0.5*x**2)*np.cos(np.pi*x)
>>> from scitools.aplotter import plot
>>> plot(x, y)
```



5.4 Plotting Difficulties

The previous examples on plotting functions demonstrate how easy it is to make graphs. Nevertheless, the shown techniques might easily fail to plot some functions correctly unless we are careful. Next we address two types of difficult functions: piecewisely defined functions and rapidly varying functions.

5.4.1 Piecewisely Defined Functions

A piecewisely defined function has different function definitions in different intervals along the x axis. The resulting function, made up of pieces, may have discontinuities in the function value or in derivatives. We have to be very careful when plotting such functions, as the next two examples will show. The problem is that the plotting mechanism draws straight lines between coordinates on the function's curve, and these straight lines may not yield a satisfactory visualization of the function. The first example has a discontinuity in the function itself at one point, while the other example has a discontinuity in the derivative at three points.

Example: The Heaviside function Let us plot the Heaviside function

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

The most natural way to proceed is first to define the function as

```
def H(x):
    return (0 if x < 0 else 1)
```

The standard plotting procedure where we define a coordinate array `x` and call `y = H(x)` will not work for array arguments `x`, of reasons to be explained in Sect. 5.5.2. However, we may use techniques from that chapter to create a function `Hv(x)` that works for array arguments. Even with such a function we face difficulties with plotting it.

Since the Heaviside function consists of two flat lines, one may think that we do not need many points along the x axis to describe the curve. Let us try with nine points:

```
x = np.linspace(-10, 10, 9)
from scitools.std import plot
plot(x, Hv(x), axis=[x[0], x[-1], -0.1, 1.1])
```

However, so few x points are not able to describe the jump from 0 to 1 at $x = 0$, as shown by the solid line in Fig. 5.8 (left). Using more points, say 50 between -10 and 10,

```
x2 = np.linspace(-10, 10, 50)
plot(x, Hv(x), 'r', x2, Hv(x2), 'b',
     legend=('5 points', '50 points'),
     axis=[x[0], x[-1], -0.1, 1.1])
```

makes the curve look better. However, the step is still not strictly vertical. More points will improve the situation. Nevertheless, the best is to draw two flat lines directly: from $(-10, 0)$ to $(0, 0)$, then to $(0, 1)$ and then to $(10, 1)$:

```
plot([-10, 0, 0, 10], [0, 0, 1, 1],
     axis=[x[0], x[-1], -0.1, 1.1])
```

The result is shown in Fig. 5.8 (right).

Some will argue that the plot of $H(x)$ should not contain the vertical line from $(0, 0)$ to $(0, 1)$, but only two horizontal lines. To make such a plot, we must draw two distinct curves, one for each horizontal line:

```
plot([-10,0], [0,0], 'r-', [0,10], [1,1], 'r-',
     axis=[x[0], x[-1], -0.1, 1.1])
```

Observe that we must specify the same line style for both lines (curves), otherwise they would by default get different colors on the screen or different line types in a hardcopy of the plot. We remark, however, that discontinuous functions like $H(x)$ are often visualized with vertical lines at the jumps, as we do in Fig. 5.8b.

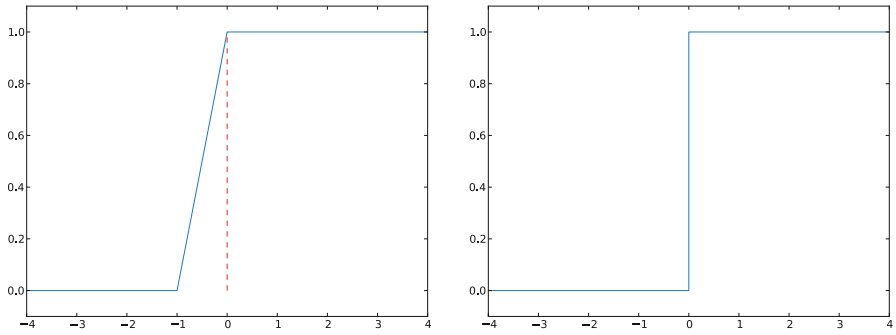


Fig. 5.8 Plot of the Heaviside function using 9 equally spaced x points (*left*) and with a double point at $x = 0$ (*right*)

Example: A hat function Let us plot the hat function $N(x)$, shown as the solid line in Fig. 5.9. This function is a piecewise linear function. The implementation of $N(x)$ must use `if` tests to locate where we are along the x axis and then evaluate the right linear piece of $N(x)$. A straightforward implementation with plain `if` tests does not work with array arguments `x`, but Sect. 5.5.3 explains how to make a vectorized version `Nv(x)` that works for array arguments as well. Anyway, both the scalar and the vectorized versions face challenges when it comes to plotting.

A first approach to plotting could be

```
x = np.linspace(-2, 4, 6)
plot(x, Nv(x), 'r', axis=[x[0], x[-1], -0.1, 1.1])
```

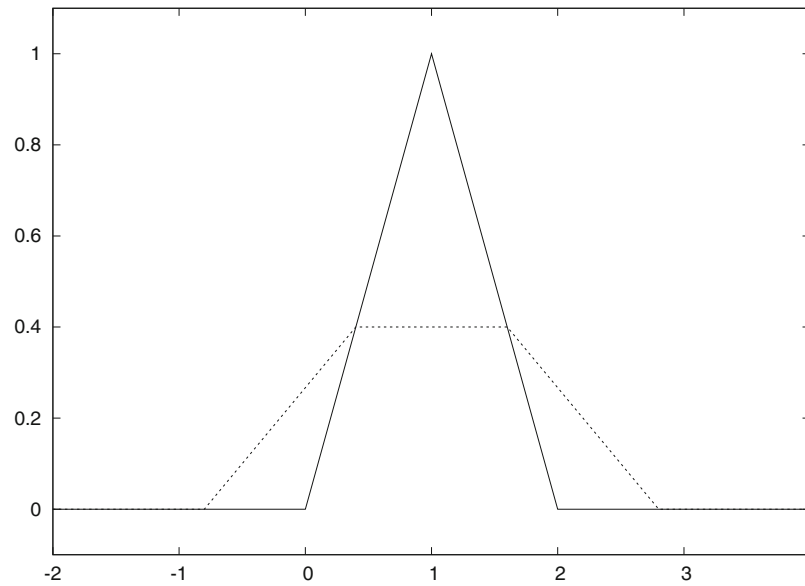


Fig. 5.9 Plot of a hat function. The solid line shows the exact function, while the dashed line arises from using inappropriate points along the x axis

This results in the dashed line in Fig. 5.9. What is the problem? The problem lies in the computation of the x vector, which does not contain the points $x = 1$ and $x = 2$ where the function makes significant changes. The result is that the hat is flattened. Making an x vector with all critical points in the function definitions, $x = 0, 1, 2$, provides the necessary remedy, either

```
x = np.linspace(-2, 4, 7)
```

or the simple

```
x = [-2, 0, 1, 2, 4]
```

Any of these x alternatives and a `plot(x, Nv(x))` will result in the solid line in Fig. 5.9, which is the correct visualization of the $N(x)$ function.

As in the case of the Heaviside function, it is perhaps best to drop using vectorized evaluations and just draw straight lines between the critical points of the function (since the function is linear):

```
x = [-2, 0, 1, 2, 4]
y = [N(xi) for xi in x]
plot(x, y, 'r', axis=[x[0], x[-1], -0.1, 1.1])
```

5.4.2 Rapidly Varying Functions

Let us now visualize the function $f(x) = \sin(1/x)$, using 10 and 1000 points:

```
def f(x):
    return sin(1.0/x)

from scitools.std import linspace, plot
x1 = linspace(-1, 1, 10)
x2 = linspace(-1, 1, 1000)
plot(x1, f(x1), label='%d points' % len(x))
plot(x2, f(x2), label='%d points' % len(x))
```

The two plots are shown in Fig. 5.10. Using only 10 points gives a completely wrong picture of this function, because the function oscillates faster and faster as we approach the origin. With 1000 points we get an impression of these oscillations, but the accuracy of the plot in the vicinity of the origin is still poor. A plot with 100000 points has better accuracy, in principle, but the extremely fast oscillations near the origin just drowns in black ink (you can try it out yourself).

Another problem with the $f(x) = \sin(1/x)$ function is that it is easy to define an x vector containing $x = 0$, such that we get division by zero. Mathematically, the $f(x)$ function has a singularity at $x = 0$: it is difficult to define $f(0)$, so one should exclude this point from the function definition and work with a domain $x \in [-1, -\epsilon] \cup [\epsilon, 1]$, with ϵ chosen small.

The lesson learned from these examples is clear. You must investigate the function to be visualized and make sure that you use an appropriate set of x coordinates along the curve. A relevant first step is to double the number of x coordinates

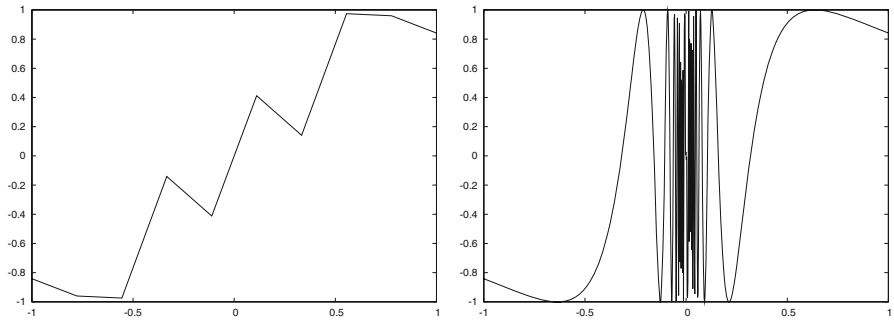


Fig. 5.10 Plot of the function $\sin(1/x)$ with 10 points (*left*) and 1000 points (*right*)

and check if this changes the plot. If not, you probably have an adequate set of x coordinates.

5.5 More Advanced Vectorization of Functions

So far we have seen that vectorization of a Python function `f(x)` implementing some mathematical function $f(x)$ seems trivial: `f(x)` works right away with an array argument `x` and, in that case, returns an array where f is applied to each element in `x`. When the expression for $f(x)$ is given in terms of a string and the `StringFunction` tool is used to generate the corresponding Python function `f(x)`, one extra step must be performed to vectorize the Python function. This step is explained in Sect. 5.5.1.

The described vectorization works well as long as the expression $f(x)$ is a mathematical formula without any `if` test. As soon as we have `if` tests (conditional mathematical expressions) the vectorization becomes more challenging. Some useful techniques are explained through two examples in Sects. 5.5.2 and 5.5.3. The described techniques are considered advanced material and only necessary when the time spent on evaluating a function at a very large set of points needs to be significantly decreased.

5.5.1 Vectorization of StringFunction Objects

The `StringFunction` object from `scitools.std` can convert a formula, available as a string, to a callable Python function (see Sect. 4.3.3). However, the function cannot work with array arguments unless we explicitly tell the `StringFunction` object to do so. The recipe is very simple. Say `f` is some `StringFunction` object. To allow array arguments we are required to call `f.vectorize(globals())` once:

```
from numpy import *
x = linspace(0, 1, 30)
# f(x) will in general not work

f.vectorize(globals())
values = f(x)            # f works with array arguments
```

It is important that you import everything from `numpy` (or `scitools.std`) *before* calling `f.vectorize`, exactly as shown.

You may take the `f.vectorize` call as a magic recipe. Still, some readers want to know what problem `f.vectorize` solves. Inside the `StringFunction` module we need to have access to mathematical functions for expressions like `sin(x)*exp(x)` to be evaluated. These mathematical functions are by default taken from the `math` module and hence they do not work with array arguments. If the user, in the main program, has imported mathematical functions that work with array arguments, these functions are registered in a dictionary returned from `globals()`. By the `f.vectorize` call we supply the `StringFunction` module with the user's global namespace so that the evaluation of the string expression can make use of the mathematical functions for arrays from the user's program. Unless you use `np.sin(x)*np.cos(x)` etc. in the string formulas, make sure you do a `from numpy import *` so that the function names are defined without any prefix.

Even after calling `f.vectorize(globals())`, a `StringFunction` object may face problems with vectorization. One example is a piecewise constant function as specified by a string expression `'1 if x > 2 else 0'`. Section 5.5.2 explains why `if` tests fail for arrays and what the remedies are.

5.5.2 Vectorization of the Heaviside Function

We consider the widely used Heaviside function defined by

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

The most compact way if implementing this function is

```
def H(x):
    return (0 if x < 0 else 1)
```

Trying to call `H(x)` with an array argument `x` fails:

```
>>> def H(x): return (0 if x < 0 else 1)
...
>>> import numpy as np
>>> x = np.linspace(-10, 10, 5)
>>> x
array([-10.,  -5.,   0.,   5.,  10.])
>>> H(x)
...
ValueError: The truth value of an array with more than
one element is ambiguous. Use a.any() or a.all()
```

The problem is related to the test `x < 0`, which results in an array of boolean values, while the `if` test needs a single boolean value (essentially taking `bool(x < 0)`):

```
>>> b = x < 0
>>> b
array([ True,  True, False, False, False], dtype=bool)
>>> bool(b)  # evaluate b in a boolean context
...
ValueError: The truth value of an array with more than
one element is ambiguous. Use a.any() or a.all()
>>> b.any()  # True if any element in b is True
True
>>> b.all()  # True if all elements in b are True
False
```

The `any` and `all` calls do not help us since we want to take actions element by element depending on whether `x[i] < 0` or not.

There are four ways to find a remedy to our problems with the `if x < 0` test: (i) we can write an explicit loop for computing the elements, (ii) we can use a tool for automatically vectorize `H(x)`, (iii) we can mix boolean and floating-point calculations, or (iv) we can manually vectorize the `H(x)` function. All four methods will be illustrated next.

Loop The following function works well for arrays if we insert a simple loop over the array elements (such that `H(x)` operates on scalars only):

```
def H_loop(x):
    r = np.zeros(len(x))
    for i in xrange(len(x)):
        r[i] = H(x[i])
    return r

# Example:
x = np.linspace(-5, 5, 6)
y = H_loop(x)
```

Automatic vectorization Numerical Python contains a method for automatically vectorizing a Python function `H(x)` that works with scalars (pure numbers) as `x` argument:

```
import numpy as np
H_vec = np.vectorize(H)
```

The `H_vec(x)` function will now work with vector/array arguments `x`. Unfortunately, such automatically vectorized functions runs at a fairly slow speed compared to the implementations below (see the end of Sect. 5.5.3 for specific timings).

Mixing boolean and floating-point calculations It appears that a very simple solution to vectorizing the `H(x)` function is to implement it as

```
def H(x):
    return x >= 0
```

The return value is now a `bool` object, not an `int` or `float` as we would mathematically expect to be the proper type of the result. However, the `bool` object works well in both scalar and vectorized operations as long as we involve the returned `H(x)` in some arithmetic expression. The `True` and `False` values are then interpreted as 1 and 0. Here is a demonstration:

```
>>> x = np.linspace(-1, 1, 5)
>>> H(x)
array([False, False,  True,  True,  True], dtype=bool)
>>> 1*H(x)
array([0, 0, 1, 1, 1])
>>> H(x) - 2
array([-2, -2, -1, -1, -1])
>>>
>>> x = 0.2   # test scalar argument
>>> H(x)
True
>>> 1*H(x)
1
>>> H(x) - 2
-1
```

If returning a boolean value is considered undesirable, we can turn the `bool` object into the proper type by

```
def H(x):
    r = x >= 0
    if isinstance(x, (int,float)):
        return int(r)
    elif isinstance(x, np.ndarray):
        return np.asarray(r, dtype=np.int)
```

Manual vectorization By manual vectorization we normally mean translating the algorithm into a set of calls to functions in the `numpy` package such that no loops are visible in the Python code. The last version of the `H(x)` is a manual vectorization, but now we shall look at a more general technique when the result is not necessarily 0 or 1. In general, manual vectorization is non-trivial and requires knowledge of and experience with the underlying library for array computations. Fortunately, there is a simple `numpy` recipe for turning functions of the form

```
def f(x):
    if condition:
        r = <expression1>
    else:
        r = <expression2>
    return r
```

into vectorized form:

```
def f_vectorized(x):
    x1 = <expression1>
    x2 = <expression2>
```

```
    r = np.where(condition, x1, x2)
    return r
```

The `np.where` function returns an array of the same length as `condition`, whose element no. `i` equals `x1[i]` if `condition[i]` is `True`, and `x2[i]` otherwise. With Python loops we can express this principle as

```
def my_where(condition, x1, x2):
    r = np.zeros(len(condition))   # result
    for i in xrange(condition):
        r[i] = x1[i] if condition[i] else x2[i]
    return r
```

The `x1` and `x2` variables can be pure numbers too in the call to `np.where`.

In our case we can use the `np.where` function as follows:

```
def Hv(x):
    return np.where(x < 0, 0.0, 1.0)
```

Instead of using `np.where` we can apply *boolean indexing*. The idea is that an array `a` allows to be indexed by an array `b` of boolean values: `a[b]`. The result `a[b]` is a new array with all the elements `a[i]` where `b[i]` is `True`:

```
>>> a
array([  0. ,   2.5,   5. ,   7.5,  10. ])
>>> b = a > 5
>>> b
array([False, False, False,  True,  True], dtype=bool)
>>> a[b]
array([  7.5,  10. ])
```

We can assign new values to the elements in `a` where `b` is `True`:

```
>>> a[b]
array([  7.5,  10. ])
>>> a[b] = np.array([-10, -20], dtype=np.float)
>>> a
array([  0. ,   2.5,   5. , -10. , -20. ])
>>> a[b] = -4
>>> a
array([ 0. ,  2.5,  5. , -4. , -4. ])
```

To implement the Heaviside function, we start with an array of zeros and then assign 1 to the elements where `x >= 0`:

```
def Hv(x):
    r = np.zeros(len(x), dtype=np.int)
    r[x >= 0] = 1
    return r
```

5.5.3 Vectorization of a Hat Function

We now turn the attention to the hat function $N(x)$ defined by

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

The corresponding Python implementation `N(x)` is

```
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
```

Unfortunately, this `N(x)` function does not work with array arguments `x`, because the boolean expressions, like `x < 0`, are arrays and they cannot yield a single `True` or `False` value for the `if` tests, as explained in Sect. 5.5.2.

The simplest remedy is to use `np.vectorize` from Sect. 5.5.2:

```
N_vec = np.vectorize(N)
```

It is then important that `N(x)` returns `float` and not `int` values, otherwise the vectorized version will produce `int` values and hence be incorrect.

A manual rewrite, yielding a faster vectorized function, is more demanding than for the Heaviside function because we now have multiple branches in the `if` test. One sketch is to replace

```
if condition1:
   r = <expression1>
elif condition2:
   r = <expression2>
elif condition3:
   r = <expression3>
else:
   r = <expression4>
```

by

```
x1 = <expression1>
x2 = <expression2>
x3 = <expression3>
x4 = <expression4>
r = np.where(condition1, x1, x4)  # initialize with "else" expr.
r = np.where(condition2, x2, r)
r = np.where(condition3, x3, r)
```

Alternatively, we can use boolean indexing. Assuming that `<expressionX>` is some expression involving an array `x` and coded as a Python function `fX(x)` (`X` is 1, 2, 3, or 4), we can write

```
r = f4(x)
r[condition1] = f1(x[condition1])
r[condition2] = f2(x[condition2])
r[condition3] = f2(x[condition3])
```

Specifically, when the function for scalar arguments `x` reads

```
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
```

a vectorized attempt would be

```
def Nv(x):
    r = np.where(x < 0,      0.0,  0.0)
    r = np.where(0 <= x < 1, x,    r)
    r = np.where(1 <= x < 2, 2-x,  r)
    r = np.where(x >= 2,     0.0,  r)
    return r
```

The first and last line are not strictly necessary as we could just start with a zero vector (making the insertion of zeros for the first and last condition a redundant operation).

However, any condition like `0 <= x < 1`, which is equivalent to `0 <= x and x < 1`, does not work because the `and` operator does not work with array arguments. Fortunately, there is a simple solution to this problem: the function `logical_and` in `numpy`. A working `Nv` function must apply `logical_and` instead in each condition:

```
def Nv1(x):
    condition1 = x < 0
    condition2 = np.logical_and(0 <= x, x < 1)
    condition3 = np.logical_and(1 <= x, x < 2)
    condition4 = x >= 2

    r = np.where(condition1, 0.0, 0.0)
    r = np.where(condition2, x,   r)
    r = np.where(condition3, 2-x, r)
    r = np.where(condition4, 0.0, r)
    return r
```

With boolean indexing we get the alternative form

```
def Nv2(x):
    condition1 = x < 0
    condition2 = np.logical_and(0 <= x, x < 1)
    condition3 = np.logical_and(1 <= x, x < 2)
    condition4 = x >= 2

    r = np.zeros(len(x))
    r[condition1] = 0.0
    r[condition2] = x[condition2]
    r[condition3] = 2-x[condition3]
    r[condition4] = 0.0
    return r
```

Again, the first and last assignment to `r` can be omitted in this special case where we start with a zero vector.

The file `hat.py` implements four vectorized versions of the `N(x)` function: `N_loop`, which is a plain loop calling up `N(x)` for each `x[i]` element in the array `x`; `N_vec`, which is the result of automatic vectorization via `np.vectorize`; the `Nv1` function shown above, which uses the `np.where` constructions; and the `Nv2` function, which uses boolean indexing. With a length of `x` of 1,000,000, the results on my computer (MacBook Air 11", 2 1.6GHz Intel CPU, running Ubuntu 12.04 in a VMWare virtual machine) became 4.8 s for `N_loop`, 1 s `N_vec`, 0.3 s for `Nv1`, and 0.08 s for `Nv2`. Boolean indexing is clearly the fastest method.

5.6 More on Numerical Python Arrays

This section lists some more advanced but useful operations with Numerical Python arrays.

5.6.1 Copying Arrays

Let `x` be an array. The statement `a = x` makes `a` refer to the same array as `x`. Changing `a` will then also affect `x`:

```
>>> import numpy as np
>>> x = np.array([1, 2, 3.5])
>>> a = x
>>> a[-1] = 3  # this changes x[-1] too!
>>> x
array([ 1.,  2.,  3.])
```

Changing `a` without changing `x` requires `a` to be a copy of `x`:

```
>>> a = x.copy()
>>> a[-1] = 9
>>> a
array([ 1.,  2.,  9.])
>>> x
array([ 1.,  2.,  3.])
```

5.6.2 In-Place Arithmetics

Let `a` and `b` be two arrays of the same shape. The expression `a += b` means `a = a + b`, but this is not the complete story. In the statement `a = a + b`, the sum `a + b` is first computed, yielding a new array, and then the name `a` is bound to this new array. The old array `a` is lost unless there are other names assigned to this array. In the statement `a += b`, elements of `b` are added directly into the elements of `a` (in memory). There is no hidden intermediate array as in `a = a + b`. This implies that `a += b` is more efficient than `a = a + b` since Python avoids making an extra array. We say that the operators `+=`, `*=`, and so on, perform *in-place* arithmetics in arrays.

Consider the compound array expression

```
a = (3*x**4 + 2*x + 4)/(x + 1)
```

The computation actually goes as follows with seven hidden arrays for storing intermediate results:

- `r1 = x**4`
- `r2 = 3*r1`
- `r3 = 2*x`
- `r4 = r2 + r3`
- `r5 = r4 + 4`
- `r6 = x + 1`
- `r7 = r5/r6`
- `a = r7`

With in-place arithmetics we can get away with creating three new arrays, at a cost of a significantly less readable code:

```
a = x.copy()
a **= 4
a *= 3
a += 2*x
a += 4
a /= x + 1
```

The three extra arrays in this series of statement arise from copying `x`, and computing the right-hand sides `2*x` and `x+1`.

Quite often in computational science and engineering, a huge number of arithmetics is performed on very large arrays, and then saving memory and array allocation time by doing in-place arithmetics is important.

The mix of assignment and in-place arithmetics makes it easy to make unintended changes of more than one array. For example, this code changes `x`:

```
a = x
a += y
```

since `a` refers to the same array as `x` and the change of `a` is done in-place.

5.6.3 Allocating Arrays

We have already seen that the `np.zeros` function is handy for making a new array `a` of a given size. Very often the size and the type of array elements have to match another existing array `x`. We can then either copy the original array, e.g.,

```
a = x.copy()
```

and fill elements in `a` with the right new values, or we can say

```
a = np.zeros(x.shape, x.dtype)
```

The attribute `x.dtype` holds the array element type (`dtype` for data type), and `x.shape` is a tuple with the array dimensions. The variable `a.ndim` holds the number of dimensions.

Sometimes we may want to ensure that an object is an array, and if not, turn it into an array. The `np.asarray` function is useful in such cases:

```
a = np.asarray(a)
```

Nothing is copied if `a` already is an array, but if `a` is a list or tuple, a new array with a copy of the data is created.

5.6.4 Generalized Indexing

Section 5.2.2 shows how slices can be used to extract and manipulate subarrays. The slice `f:t:i` corresponds to the index set `f, f+i, f+2*i, ...` up to, but not including, `t`. Such an index set can be given explicitly too: `a[range(f,t,i)]`. That is, the integer list from `range` can be used as a set of indices. In fact, any integer list or integer array can be used as index:

```
>>> a = np.linspace(1, 8, 8)
>>> a
array([ 1.,  2.,  3.,  4.,  5.,  6.,  7.,  8.])
>>> a[[1,6,7]] = 10
>>> a
array([  1.,  10.,   3.,   4.,   5.,   6.,  10.,  10.])
>>> a[range(2,8,3)] = -2   # same as a[2:8:3] = -2
>>> a
array([  1.,  10.,  -2.,   4.,   5.,  -2.,  10.,  10.])
```

We can also use boolean arrays to generate an index set. The indices in the set will correspond to the indices for which the boolean array has `True` values. This functionality allows expressions like `a[x<m]`. Here are two examples, continuing the previous interactive session:

```
>>> a[a < 0]            # pick out the negative elements of a
array([-2., -2.])
>>> a[a < 0] = a.max()
>>> a
array([  1.,  10.,  10.,   4.,   5.,  10.,  10.,  10.])
>>> # Replace elements where a is 10 by the first
>>> # elements from another array/list:
>>> a[a == 10] = [10, 20, 30, 40, 50, 60, 70]
>>> a
array([  1.,  10.,  20.,   4.,   5.,  30.,  40.,  50.])
```

Generalized indexing using integer arrays or lists is important for vectorized initialization of array elements. The syntax for generalized indexing of higher-dimensional arrays is slightly different, see Sect. 5.8.2.

5.6.5 Testing for the Array Type

Inside an interactive Python shell you can easily check an object's type using the `type` function (see Sect. 1.5.2). In case of a Numerical Python array, the type name is `ndarray`:

```
>>> a = np.linspace(-1, 1, 3)
>>> a
array([-1.,  0.,  1.])
>>> type(a)
<type 'numpy.ndarray'>
```

Sometimes you need to test if a variable is an `ndarray` or a `float` or `int`. The `isinstance` function can be used this purpose:

```
>>> isinstance(a, np.ndarray)
True
>>> isinstance(a, (float,int))  # float or int?
False
```

A typical use of `isinstance` and `type` to check on object's type is shown next.

Example: Vectorizing a constant function Suppose we have a constant function,

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

This function accepts an array argument `x`, but will return a `float` while a vectorized version of the function should return an array of the same shape as `x` where each element has the value 2. The vectorized version can be realized as

```
def fv(x):
    return np.zeros(x.shape, x.dtype) + 2
```

The optimal vectorized function would be one that works for both a scalar and an array argument. We must then test on the argument type:

```
def f(x):
    if isinstance(x, (float, int)):
        return 2
    elif isinstance(x, np.ndarray):
        return np.zeros(x.shape, x.dtype) + 2
    else:
        raise TypeError\
        ('x must be int, float or ndarray, not %s' % type(x))
```

5.6.6 Compact Syntax for Array Generation

There is a special compact syntax `r_[f:t:s]` for the `linspace` function:

```
>>> a = r_[-5:5:11j]  # same as linspace(-5, 5, 11)
>>> print a
[-5. -4. -3. -2. -1.  0.  1.  2.  3.  4.  5.]
```

Here, `11j` means 11 coordinates (between -5 and 5, including the upper limit 5). That is, the number of elements in the array is given with the imaginary number syntax.

5.6.7 Shape Manipulation

The `shape` attribute in array objects holds the shape, i.e., the size of each dimension. A function `size` returns the total number of elements in an array. Here are a few equivalent ways of changing the shape of an array:

```
>>> a = np.linspace(-1, 1, 6)
>>> print a
[-1.  -0.6 -0.2  0.2  0.6  1. ]
>>> a.shape
(6,)
>>> a.size
6
>>> a.shape = (2, 3)
>>> a = a.reshape(2, 3)    # alternative
>>> a.shape
(2, 3)
>>> print a
[[-1.  -0.6 -0.2]
 [ 0.2  0.6  1. ]]
>>> a.size                 # total no of elements
6
>>> len(a)                 # no of rows
2
>>> a.shape = (a.size,)    # reset shape
```

Note that `len(a)` always returns the length of the first dimension of an array.

5.7 High-Performance Computing with Arrays

Programs with lots of array calculations may soon consume much time and memory, so it may quickly become crucial to speed up calculations and use as little memory as possible. The main technique for speeding up array calculations is vectorization, i.e., avoiding explicit loops in Python over array elements. To save memory usage, one needs to understand when arrays get allocated and avoid this by in-place array arithmetics. You should review Sect. 5.6.2 about array allocation and in-place arithmetics before reading on.

Example: `axpy` Our computational case study concerns the famous "axpy" operation: $r = ax + y$, where a is a number and x and y are arrays. All implementations and the associated experimentation are found in the file `hpc_axpy.py`.

5.7.1 Scalar Implementation

A naive loop implementation of the "axpy" operation $ax + y$ reads

```
def axpy_loop_newr(a, x, y):
    r = np.zeros_like(x)
    for i in range(r.size):
        r[i] = a*x[i] + y[i]
    return r
```

Classical implementations overwrite y by $ax + y$: $y \leftarrow ax + y$, but we shall make implementations where we either can overwrite y or place $ax + y$ in another array. The function above creates a new array for the result.

Rather than allocating the array inside the function, we can put that burden on the user and provide a result array `r` as input:

```
def axpy_loop(a, x, y, r):
    for i in range(r.size):
        r[i] = a*x[i] + y[i]
    return r
```

The advantage of this version is that we can either overwrite y by $ax + y$ or store $ax + y$ in a separate array:

```
# Classical axpy
y = axpy_loop(a, x, y, y)

# Store axpy result in separate array
r = np.zeros_like(x)
r = axpy_loop(a, x, y, r)
```

Python functions return output data

The call

```
r = axpy_loop(a, x, y, r)
```

can equally well be written

```
axpy_loop(a, x, y, r)
```

This is the typical coding style in Fortran, C, or C++ (where `r` is then transferred as a reference or pointer to the array data). In Python, there is no need for the function `axpy_loop` to return `r`, because the assignment to `r[i]` inside the loop changes all elements of the `r`. The array `r` will therefore be modified after calling `axpy_loop(a, x, y, r)` anyway. However, it is a good convention in Python that *all input data to a function are arguments and all output data are returned*. With

```
r = axpy_loop(a, x, y, r)
```

we clearly see that `r` is both input and output.

5.7.2 Vectorized Implementation

The vectorized implementation of the "axpy" operation reads

```
def axpy1(a, x, y):
    r = a*x + y
    return r
```

Note that the result is placed in a new array arrising from the operation `a*x+y`. The speed up of vectorization is significant, see Fig. 5.11 (made by the function `effect_of_vec` in the file `hpc_axpy.py`).

Temporary arrays are needed in the vectorized implementation. One would expect that `a*x` must be calculated and stored in a temporary array, call it `r1`, and then `r1 + y` must be evaluated and stored in another allocated array `r`, which is returned. It appears that `a*x + y` only needs the allocation of one array, the one to be returned (we have investigated the memory consumption in detail using the `memory_profiler` module). Anyway, repeated calls to `axpy1` with large arrays lead to an allocation of a new large array in each call.

5.7.3 Memory-Saving Implementation

Applications with large arrays should avoid unnecessary allocation of temporary arrays and instead reuse pre-allocated arrays. Suppose we have allocated an array for the result `r = ax + y` once and for all. We can pass the `r` array to the computing function as in the `axpy_loop` function above and use the memory in `r` for intermediate calculation. In vectorized code, this requires use of *in-place* array arithmetics (see Sect. 5.6.2)

In-place arithmetics for doing `r = a*x + y` in a pre-allocated array `r` will first copy all elements of `x` into `r`, then perform elementwise multiplication by `a`, and finally elementwise addition of `y`:

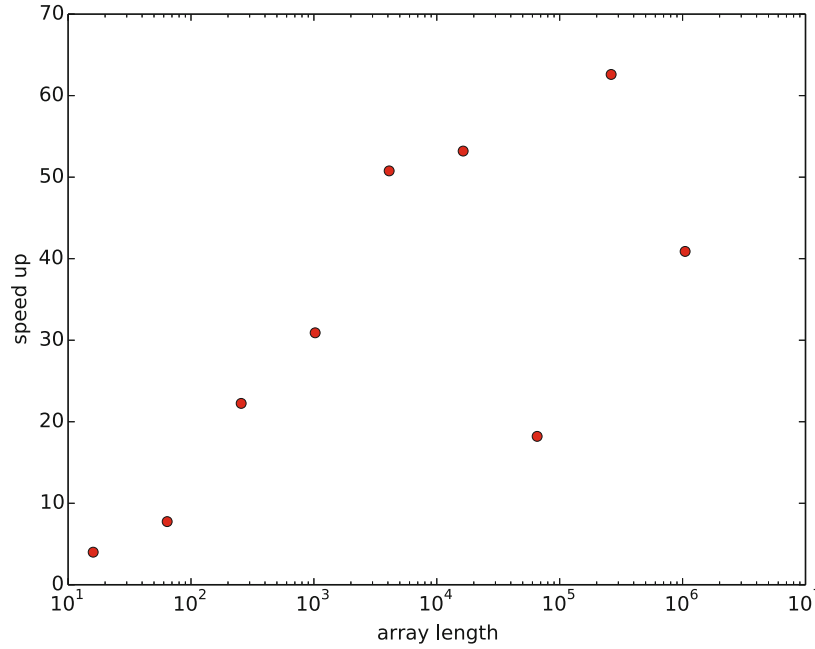


Fig. 5.11 Improved efficiency of vectorizing the "axpy" operation as function of array length

```
def axpy2(a, x, y, r):
    r[:] = x
    r *= a
    r += y
    return r
```

Note that `r[:] = x` inserts the elements of `x` into `r`. A mathematically equivalent construction, `r = x.copy()`, allocates a new object and fills it with the values of `x` before the name `r` refers to this object. The array `r` supplied as argument to the function is then lost, and the returned array is another object.

We can perform repeated calls to the `axpy2` function without any extra memory allocation. This can be proved by a small code snippet where we use `id(r)` to see the unique identity of the `r` array. If this identity remains constant through calls, we always reuse the pre-allocated `r` array:

```
r = np.zeros_like(x)
print id(r)
for i in range(10):
    r = axpy2(a, x, y, r)
    print id(r)
```

The output prints the same number, proving that it is physically the same object we feed as `r` to `axpy2` that is also returned.

We can equally well drop returning `r` and utilize that the changes made by in-place arithmetics is always reflected in the `r` array we allocate outside the function:

```
def axpy3(a, x, y, r):
    r[:] = x
    r *= a
    r += y
```

The call can now just be

```
axpy3(a, x, y, r)
```

However, as emphasized in Sect. 5.7.1, in Python we usually return the output data (because this is no extra cost, only references to objects are physically transferred back to the calling code).

5.7.4 Analysis of Memory Usage

The module `memory_profiler` is very useful for analyzing the memory usage of every statement in a program. The module is installed by

Terminal

```
Terminal> sudo pip install memory_profiler
```

Each function we want to analyze must have (the decorator) `@profile` at the line above, e.g.,

```
@profile
def axpy1(a, x, y:
    r = a*x + y
    return r
```

We can then run a program with name `axpy.py` by

Terminal

```
Terminal> python -m memory_profiler axpy.py
```

The arrays must be quite large to see a significant increase in memory usage. With 10,000,000 elements in each array we get output like

```
Line #    Mem usage    Increment   Line Contents
================================================
     1  251.977 MiB    0.000 MiB   @profile
     2                              def axpy1(a, x, y:
     3  328.273 MiB   76.297 MiB       r = a*x + y
     4  328.273 MiB    0.000 MiB       return r
```

```
Line #    Mem usage    Increment   Line Contents
================================================
     6  251.977 MiB    0.000 MiB   @profile
     7                              def axpy2(a, x, y, r):
     8  251.977 MiB    0.000 MiB       r[:] = x
     9  251.977 MiB    0.000 MiB       r *= a
    10  251.977 MiB    0.000 MiB       r += y
    11  251.977 MiB    0.000 MiB       return r
```

This demonstrates the larger memory consumption of `axpy1` compared with `axpy2`.

5.7.5 Analysis of the CPU Time

The module `line_profiler` can time each line of a program. Installation is easily done by `sudo pip install line_profiler`. As for `module_profiler` described in the previous section, also `line_profiler` requires each function to be analyzed to have (the decorator) `@profile` at the line above the function. The module is installed together with an analysis script `kernprof` that we use to run the program:

Terminal

```
Terminal> kernprof -l -v axpy.py
```

With an array length of 500,000 we get output like

```
Total time: 0.014291 s
Function: axpy1 at line 1

Line #  Hits     Time  Per Hit   % Time  Line Contents
==============================================================
 1                                       @profile
 2                                       def axpy1(a, x, y):
 3     3        14283   4761.0     99.9      r = a*x + y
 4     3            8      2.7      0.1      return r

Total time: 0.004382 s
Function: axpy2 at line 6

Line #  Hits  Time  Per Hit   % Time  Line Contents
==============================================================
 6                                      @profile
 7                                      def axpy2(a, x, y, r):
 8     3      1981    660.3     45.2      r[:] = x
 9     3      1258    419.3     28.7      r *= a
10     3      1138    379.3     26.0      r += y
11     3         5      1.7      0.1      return r

Total time: 1.38674 s
Function: axpy_loop at line 26
```

```
Line #  Hits    Time Per Hit  % Time  Line Contents
==============================================================
26                                    @profile
27                                    def axpy_loop(a, x, y, r):
28   1500006  449747     0.3    32.4      for i in range(r.size):
29   1500003  936985     0.6    67.6          r[i] = a*x[i] + y[i]
30         3      10     3.3     0.0      return r
```

We see that the administration of the for loop takes 1/3 of the total cost of the loop.

Both `line_profiler` and `memory_profiler` are very useful tools for spotting inefficient constructions in a code.

5.8 Higher-Dimensional Arrays

5.8.1 Matrices and Arrays

Vectors appeared when mathematicians needed to calculate with a list of numbers. When they needed a table (or a list of lists in Python terminology), they invented the concept of *matrix* (singular) and *matrices* (plural). A table of numbers has the numbers ordered into rows and columns. One example is

$$\begin{bmatrix} 0 & 12 & -1 & 5 \\ -1 & -1 & -1 & 0 \\ 11 & 5 & 5 & -2 \end{bmatrix}$$

This table with three rows and four columns is called a 3×4 matrix (mathematicians may not like this sentence, but it suffices for our purposes). If the symbol A is associated with this matrix, $A_{i,j}$ denotes the number in row number i and column number j. Counting rows and columns from 0, we have, for instance, $A_{0,0} = 0$ and $A_{2,3} = -2$. We can write a general $m \times n$ matrix A as

$$\begin{bmatrix} A_{0,0} & \cdots & A_{0,n-1} \\ \vdots & \ddots & \vdots \\ A_{m-1,0} & \cdots & A_{m-1,n-1} \end{bmatrix}$$

Matrices can be added and subtracted. They can also be multiplied by a scalar (a number), and there is a concept of length or size. The formulas are quite similar to those presented for vectors, but the exact form is not important here.

We can generalize the concept of table and matrix to *array*, which holds quantities with in general d indices. Equivalently we say that the array has rank d. For $d = 3$, an array A has elements with three indices: $A_{p,q,r}$. If p goes from 0 to n_p-1, q from 0 to $n_q - 1$, and r from 0 to $n_r - 1$, the A array has $n_p \times n_q \times n_r$ elements in total. We may speak about the *shape* of the array, which is a d-vector holding the number of elements in each "array direction", i.e., the number of elements for each index. For the mentioned A array, the shape is (n_p, n_q, n_r).

The special case of $d = 1$ is a vector, and $d = 2$ corresponds to a matrix. When we program we may skip thinking about vectors and matrices (if you are not so

familiar with these concepts from a mathematical point of view) and instead just work with arrays. The number of indices corresponds to what is convenient in the programming problem we try to solve.

5.8.2 Two-Dimensional Numerical Python Arrays

Consider a nested list `table` of two-pairs `[C, F]` (see Sect. 2.4) constructed by

```
>>> Cdegrees = [-30 + i*10 for i in range(3)]
>>> Fdegrees = [9./5*C + 32 for C in Cdegrees]
>>> table = [[C, F] for C, F in zip(Cdegrees, Fdegrees)]
>>> print table
[[-30, -22.0], [-20, -4.0], [-10, 14.0]]
```

This nested list can be turned into an array,

```
>>> table2 = np.array(table)
>>> print table2
[[-30. -22.]
 [-20.  -4.]
 [-10.  14.]]
>>> type(table2)
<type 'numpy.ndarray'>
```

We say that `table2` is a *two-dimensional* array, or an array of rank 2.

The `table` list and the `table2` array are stored very differently in memory. The `table` variable refers to a list object containing three elements. Each of these elements is a reference to a separate list object with two elements, where each element refers to a separate `float` object. The `table2` variable is a reference to a single array object that again refers to a consecutive sequence of bytes in memory where the six floating-point numbers are stored. The data associated with `table2` are found in one chunk in the computer's memory, while the data associated with `table` are scattered around in memory. On today's machines, it is much more expensive to find data in memory than to compute with the data. Arrays make the data fetching more efficient, and this is major reason for using arrays. However, this efficiency gain is only present for very large arrays, not for a 3×2 array.

Indexing a nested list is done in two steps, first the outer list is indexed, giving access to an element that is another list, and then this latter list is indexed:

```
>>> table[1][0]     # table[1] is [-20,4], whose index 0 holds -20
-20
```

This syntax works for two-dimensional arrays too:

```
>>> table2[1][0]
-20.0
```

but there is another syntax that is more common for arrays:

```
>>> table2[1,0]
-20.0
```

A two-dimensional array reflects a table and has a certain number of rows and columns. We refer to rows as the *first dimension* of the array and columns as the *second dimension*. These two dimensions are available as `table2.shape`:

```
>>> table2.shape
(3, 2)
```

Here, 3 is the number of rows and 2 is the number of columns.

A loop over all the elements in a two-dimensional array is usually expressed as two *nested* `for` loops, one for each index:

```
>>> for i in range(table2.shape[0]):
...     for j in range(table2.shape[1]):
...         print 'table2[%d,%d] = %g' % (i, j, table2[i,j])
...
table2[0,0] = -30
table2[0,1] = -22
table2[1,0] = -20
table2[1,1] = -4
table2[2,0] = -10
table2[2,1] = 14
```

An alternative (but less efficient) way of visiting each element in an array with any number of dimensions makes use of a single `for` loop:

```
>>> for index_tuple, value in np.ndenumerate(table2):
...     print 'index %s has value %g' % \
...           (index_tuple, table2[index_tuple])
...
index (0,0) has value -30
index (0,1) has value -22
index (1,0) has value -20
index (1,1) has value -4
index (2,0) has value -10
index (2,1) has value 14
```

In the same way as we can extract sublists of lists, we can extract subarrays of arrays using slices.

```
table2[0:table2.shape[0], 1]  # 2nd column (index 1)
array([-22.,  -4.,  14.])

>>> table2[0:, 1]             # same
array([-22.,  -4.,  14.])

>>> table2[:, 1]              # same
array([-22.,  -4.,  14.])
```

To illustrate array slicing further, we create a bigger array:

```
>>> t = np.linspace(1, 30, 30).reshape(5, 6)
>>> t
array([[  1.,   2.,   3.,   4.,   5.,   6.],
       [  7.,   8.,   9.,  10.,  11.,  12.],
       [ 13.,  14.,  15.,  16.,  17.,  18.],
       [ 19.,  20.,  21.,  22.,  23.,  24.],
       [ 25.,  26.,  27.,  28.,  29.,  30.]])

>>> t[1:-1:2, 2:]
array([[  9.,  10.,  11.,  12.],
       [ 21.,  22.,  23.,  24.]])
```

To understand the slice, look at the original `t` array and pick out the two rows corresponding to the first slice `1:-1:2`,

```
       [  7.,   8.,   9.,  10.,  11.,  12.]
       [ 19.,  20.,  21.,  22.,  23.,  24.]
```

Among the rows, pick the columns corresponding to the second slice `2:`,

```
       [  9.,  10.,  11.,  12.]
       [ 21.,  22.,  23.,  24.]
```

Another example is

```
>>> t[:-2, :-1:2]
array([[  1.,   3.,   5.],
       [  7.,   9.,  11.],
       [ 13.,  15.,  17.]])
```

Generalized indexing as described for one-dimensional arrays in Sect. 5.6.4 requires a more comprehensive syntax for higher-dimensional arrays. Say we want to extract a subarray of `t` that consists of the rows with indices 0 and 3 and the columns with indices 1 and 2:

```
>>> t[np.ix_([0,3], [1,2])]
array([[  2.,   3.],
       [ 20.,  21.]])
>>> t[np.ix_([0,3], [1,2])] = 0
>>> t
array([[  1.,   0.,   0.,   4.,   5.,   6.],
       [  7.,   8.,   9.,  10.,  11.,  12.],
       [ 13.,  14.,  15.,  16.,  17.,  18.],
       [ 19.,   0.,   0.,  22.,  23.,  24.],
       [ 25.,  26.,  27.,  28.,  29.,  30.]])
```

Recall that slices only gives a view to the array, not a copy of the values:

```
>>> a = t[1:-1:2, 1:-1]
>>> a
array([[  8.,   9.,  10.,  11.],
       [  0.,   0.,  22.,  23.]])
```

```
>>> a[:,:] = -99
>>> a
array([[-99., -99., -99., -99.],
       [-99., -99., -99., -99.]])
>>> t  # is t changed to? yes!
array([[  1.,   0.,   0.,   4.,   5.,   6.],
       [  7., -99., -99., -99., -99.,  12.],
       [ 13.,  14.,  15.,  16.,  17.,  18.],
       [ 19., -99., -99., -99., -99.,  24.],
       [ 25.,  26.,  27.,  28.,  29.,  30.]])
```

5.8.3 Array Computing

The operations on vectors in Sect. 5.1.3 can quite straightforwardly be extended to arrays of any dimension. Consider the definition of applying a function $f(v)$ to a vector v: we apply the function to each element v_i in v. For a two-dimensional array A with elements $A_{i,j}$, $i = 0, \ldots, m$, $j = 0, \ldots, n$, the same definition yields

$$f(A) = (f(A_{0,0}), \ldots, f(A_{m-1,0}), f(A_{1,0}), \ldots, f(A_{m-1,n-1})) .$$

For an array B with any rank, $f(B)$ means applying f to each array entry.

The asterisk operation from Sect. 5.1.3 is also naturally extended to arrays: $A * B$ means multiplying an element in A by the corresponding element in B, i.e., element (i, j) in $A * B$ is $A_{i,j} B_{i,j}$. This definition naturally extends to arrays of any rank, provided the two arrays have the same shape.

Adding a scalar to an array implies adding the scalar to each element in the array. Compound expressions involving arrays, e.g., $\exp(-A^2) * A + 1$, work as for vectors. One can in fact just imagine that all the array elements are stored after each other in a long vector (this is actually the way the array elements are stored in the computer's memory), and the array operations can then easily be defined in terms of the vector operations from Sect. 5.1.3.

Remark Readers with knowledge of matrix computations may get confused by the meaning of A^2 in matrix computing and A^2 in array computing. The former is a matrix-matrix product, while the latter means squaring all elements of A. Which rule to apply, depends on the context, i.e., whether we are doing linear algebra or vectorized arithmetics. In mathematical typesetting, A^2 can be written as AA, while the array computing expression A^2 can be alternatively written as $A * A$. In a program, `A*A` and `A**2` are identical computations, meaning squaring all elements (array arithmetics). With NumPy arrays the matrix-matrix product is obtained by `dot(A, A)`. The matrix-vector product Ax, where x is a vector, is computed by `dot(A, x)`. However, with matrix objects (see Sect. 5.8.4) `A*A` implies the mathematical matrix multiplication AA.

We shall leave this subject of notational confusion between array computing and linear algebra here since this book will not further understanding and the confusion is seldom serious in program code if one has a good overview of the mathematics that is to be carried out.

5.8.4 Matrix Objects

This section only makes sense if you are familiar with basic linear algebra and the matrix concept. The arrays created so far have been of type `ndarray`. NumPy also has a matrix type called `matrix` or `mat` for one- and two-dimensional arrays. One-dimensional arrays are then extended with one extra dimension such that they become matrices, i.e., either a row vector or a column vector:

```
>>> import numpy as np
>>> x1 = np.array([1, 2, 3], float)
>>> x2 = np.matrix(x1)          # or mat(x1)
>>> x2                          # row vector
matrix([[ 1.,  2.,  3.]])
>>> x3 = mat(x1).T              # transpose = column vector
>>> x3
matrix([[ 1.],
        [ 2.],
        [ 3.]])

>>> type(x3)
<class 'numpy.matrixlib.defmatrix.matrix'>
>>> isinstance(x3, np.matrix)
True
```

A special feature of `matrix` objects is that the multiplication operator represents the matrix-matrix, vector-matrix, or matrix-vector product as we know from linear algebra:

```
>>> A = np.eye(3)               # identity matrix
>>> A
array([[ 1.,  0.,  0.],
       [ 0.,  1.,  0.],
       [ 0.,  0.,  1.]])
>>> A = mat(A)
>>> A
matrix([[ 1.,  0.,  0.],
        [ 0.,  1.,  0.],
        [ 0.,  0.,  1.]])
>>> y2 = x2*A                   # vector-matrix product
>>> y2
matrix([[ 1.,  2.,  3.]])
>>> y3 = A*x3                   # matrix-vector product
>>> y3
matrix([[ 1.],
        [ 2.],
        [ 3.]])
```

One should note here that the multiplication operator between standard `ndarray` objects is quite different!

Readers who are familiar with MATLAB, or intend to use Python and MATLAB together, should seriously think about programming with `matrix` objects instead of `ndarray` objects, because the `matrix` type behaves quite similar to matrices

and vectors in MATLAB. Nevertheless, `matrix` cannot be used for arrays of larger dimension than two.

5.9 Some Common Linear Algebra Operations

Python has strong support for numerical linear algebra, much like the functionality found in MATLAB. Some of the most widely used operations are exemplified below.

5.9.1 Inverse, Determinant, and Eigenvalues

We start with showing how to find the inverse and the determinant of a matrix, and how to compute the eigenvalues and eigenvectors:

```
>>> import numpy as np
>>> A = np.array([[2, 0], [0, 5]], dtype=float)

>>> np.linalg.inv(A)  # inverse matrix
array([[ 0.5,  0. ],
       [ 0. ,  0.2]])

>>> np.linalg.det(A)  # determinant
9.999999999999982

>>> eig_values, eig_vectors = np.linalg.eig(A)
>>> eig_values
array([ 2.,  5.])
>>> eig_vectors
array([[ 1.,  0.],
       [ 0.,  1.]])
```

The eigenvectors are normalized to have unit lengths.

5.9.2 Products

The `np.dot` function is used for scalar or dot product as well as matrix-vector and matrix-matrix products *between array objects*:

```
>>> a = np.array([4, 0])
>>> b = np.array([0, 1])
>>> np.dot(A, a)         # matrix vector product
array([ 8.,  0.])
>>> np.dot(a, b)         # dot product between vectors
0
>>>
>>> B = np.ones((2, 2))  # 2x2 matrix with 1's
>>> np.dot(A, B)         # matrix-matrix product
array([[ 2.,  2.],
       [ 5.,  5.]])
```

Note that using the `matrix` class instead of plain arrays (see Sect. 5.8.4) allows `*` to be used as operator for matrix-vector and matrix-matrix products.

The cross product $a \times b$, between vectors a and b of length 3, is computed by

```
>>> np.cross([1, 1, 1], [0, 0, 1])
array([ 1, -1,  0])
```

Finding the angle between vectors a and b,

$$\theta = \cos^{-1}\left(\frac{a \cdot b}{||a||\,||b||}\right),$$

goes like

```
>>> np.arccos(np.dot(a, b)/(np.linalg.norm(a)*np.linalg.norm(b)))
1.5707963267948966
```

5.9.3 Norms

Various norms of matrices and vectors are well supported by NumPy. Some common examples are

```
>>> np.linalg.norm(A)        # Frobenius norm for matrices
5.3851648071345037
>>> np.sqrt(np.sum(A**2))    # Frobenius norm: direct formula
5.3851648071345037
>>> np.linalg.norm(a)        # l2 norm for vectors
4.0
```

See `pydoc numpy.linalg.norm` for information on other norms.

5.9.4 Sum and Extreme Values

The sum of all elements or of the elements in a particular row or column is computed by `np.sum`:

```
>>> np.sum(B)          # sum of all elements
2.0
>>> B.sum()            # sum of all elements; alternative syntax
2.0
>>> np.sum(B, axis=0)  # sum over index 0 (rows)
array([ 4., -2.])
>>> np.sum(B, axis=1)  # sum over index 1 (columns)
array([ 3., -1.])
```

The maximum or minimum value of an array is also often needed:

```
>>> np.max(B)          # max over all elements
3.0
>>> B.max()            # max over all elements, alt. syntax
3.0
>>> np.min(B)          # min over all elements
-4.0
>>> np.abs(B).min()    # min absolute value
1.0
```

A very frequent application of computing the minimum absolute value occurs in test functions where we want to verify a result, e.g., that $AA^{-1} = I$, where I is the identity matrix. We then want to check the smallest absolute value in $AA^{-1} - I$:

```
>>> I = np.eye(2)   # identity matrix of size 2
>>> I
array([[ 1.,  0.],
       [ 0.,  1.]])
>>> np.abs(np.dot(A, np.linalg.inv(A)) - I).max()
0.0
```

Never use == when testing real numbers!

It could be tempting to test $AA^{-1} = I$ using the syntax

```
>>> np.dot(A, np.linalg.inv(A)) == np.eye(2)
array([[ True,  True],
       [ True,  True]], dtype=bool)
```

but there are two major problems with this test:

1. the result is a boolean matrix, not suitable for an `if` test
2. using == for matrices with float elements may fail because of rounding errors

The second problem must be solved by computing differences and comparing them against small tolerances, as we did above. Here is an example where == fails:

```
>>> A = np.array([[4, 0], [0, 49]], dtype=float)
>>> np.dot(A, np.linalg.inv(A)) == np.eye(2)
array([[ True,  True],
       [ True, False]], dtype=bool)
```

(`1.0/49*49` is not exactly `1` because of rounding errors.)

The first problem is solved by using the `C.all()`, which returns one boolean variable `True` if all elements in the boolean array `C` are `True`, otherwise it returns `False`, as in the case above:

```
>>> (np.dot(A, np.linalg.inv(A)) == np.eye(2)).all()
False
```

5.9.5 Indexing

Indexing an element is done by `A[i,j]`. A row or column is extracted as

```
>>> A[0,:]  # first row
array([ 2.,  0.])
>>> A[:,1]  # second column
array([ 0.,  5.])
```

NumPy also supports multiple values for the indices via the `np.ix_` function. Here is an example where we grab row 0 and 2, then column 1:

```
>>> C = np.array([[1,2,3],[4,5,6],[7,8,9]])
>>> C[np.ix_([0,2], [1])]  # row 0 and 2, then column 1
array([[2],
       [8]])
```

You can also use the colon notation to pick out other parts of a matrix. If `C` is a 3×5-matrix,

```
C[1:3, 0:4]
```

gives a sub-matrix consisting of the two rows of `C` after the first, and the first four columns of `C` (recall that the upper limits, here `3` and `4`, are not included).

Readers familiar with MATLAB should note that the indexing may be a bit unexpected when referring to parts of a matrix: writing `C[[0, 2], [0, 2]]` one would expect entries residing in rows/columns 0 and 2, but that behavior requires in Python the `np.ix_` command:

```
>>> C = np.array([[1, 2, 3], [4, 5, 6], [7, 8, 9]])
>>> C[np.ix_([0, 2], [0, 2])]
[[1 3]
 [7 9]]
>>> # Grab row 0, 2, then column 0 from row 0 and column 2 from row 2
>>> C[[0, 2], [0, 2]]
[1 9]
```

5.9.6 Transpose and Upper/Lower Triangular Parts

The transpose of a matrix `B` is obtained by `B.T`:

```
>>> B = np.array([[1, 2], [3, -4]], dtype=float)
>>> B.T                 # the transpose
array([[ 1.,  3.],
       [ 2., -4.]])
```

NumPy has rich functionality for doing operations on array objects. For example, one can strip down a matrix to its upper or lower triangular parts:

```
>>> np.triu(B)  # upper triangular part of B
array([[ 1.,  2.],
       [ 0., -4.]])
>>> np.tril(B)  # lower triangular part of B
array([[ 1.,  0.],
       [ 3., -4.]])
```

5.9.7 Solving Linear Systems

The perhaps most frequent operation in linear algebra is the solution of systems of linear algebraic equations: $Ax = b$, where A is a coefficient matrix, b is a given right-hand side vector, and x is the solution vector. The function `np.linalg.solve(A, b)` does the job:

```
>>> A = np.array([[1, 2], [-2, 2.5]])
>>> x = np.array([-1, 1], dtype=float)  # pick a solution
>>> b = np.dot(A, x)                    # find right-hand side

>>> np.linalg.solve(A, b)               # will this compute x?
array([-1.,  1.])
```

5.9.8 Matrix Row and Column Operations

Implementing Gaussian elimination constitutes a good pedagogical example on how to perform row and column operations on a matrix. Some needed functionality is

```
A[[i, j]] = A[[j, i]]  # swap rows i and j
A[i] *= k              # multiply row i by a constant k
A[j] += k*A[i]         # add row i, multiplied by k, to row j
```

With these operations, Gaussian elimination is programmed as follows.

```
m, n = shape(A)
for j in range(n - 1):
    for i in range(j + 1, m):
        A[i,j:] -= (A[i,j]/A[j,j])*A[j,j:]
```

Note the special syntax `j:`, which refers to indices from j and up to the end of the array. More generally, when referring to an array `a` with length `n`, the following are equivalent:

```
a[0:n]
a[:n]
a[0:]
a[:]
```

In the code for Gaussian elimination, we first eliminate the entries below the diagonal in the first column, by adding a scaled version of the first row to the other rows. Then the same procedure is applied for the second row, and so on. The result is an upper triangular matrix. The code can fail if some of the entries `A[j,j]` become zero along the way. To avoid this, we can swap rows when the problem arises. The following code implements the idea and will not fail, even if some of the columns are zero.

```
def Gaussian_elimination(A):
    rank = 0
    m, n = np.shape(A)
    i = 0
    for j in range(n):
        p = np.argmax(abs(A[i:m,j]))
        if p > 0: # swap rows
            A[[i,p+i]] = A[[p+i, i]]
        if A[i,j] != 0:
            # j is a pivot column
            rank += 1
            for r in range(i+1, m):
                A[r,j:] -= (A[r,j]/A[i,j])*A[i,j:]
            i += 1
        if i > m:
            break
    return A, rank
```

Note that we stick to the habit of returning all results from a function, here the modified matrix `A` and its rank.

5.9.9 Computing the Rank of a Matrix

The rank of a matrix equals the number of pivot columns after Gaussian elimination. The variable `rank` counts these in the code above.

Due to rounding errors, the computed rank may be higher than the actual rank: the rounding errors may imply that `A[i,j] != 0` is true, even if Gaussian elimination performed in exact arithmetics gives exactly zero. Such situations can be avoided by replacing `if A[i,j] !=0:` with `if abs(A[i,j]) > tol:`, where `tol` is some small tolerance.

A more reliable way to compute the rank is to compute the singular value decomposition of `A`, and check how many of the singular values that are larger than a threshold `epsilon`:

```
>>> A = np.array([[1, 2.01], [2.01, 4.0401]])
>>> U, s, V = np.linalg.svd(A) # s are the singular values of A
# abs(s) > tol gives an array with True and False values
# s.nonzero() lists indices k so that s[k] != 0
>>> shape((abs(s) > tol).nonzero())[1]  # rank
1
>>> A, rank = Gaussian_elimination(A)
>>> rank
2
```

If you use a tolerance check on the form `if abs(A[i,j]) > 1E-10:` in the function `Gaussian_elimination`, the code will say that the rank is 1, which is the correct value also found by using the singular value decomposition.

It is known that the determinant is nonzero if and only if the rank equals the number of rows/columns. For the matrix A we used above, the determinant should thus be 0, but also here roundoff errors come into play:

```
>>> A = np.array([[1, 2.01], [2.01, 4.0401]])
>>> A[0, 0]*A[1, 1] - A[0, 1]*A[1, 0]
8.881784197e-16
>>> np.linalg.det(A)
8.92619311799e-16
```

Using our own Gaussian elimination function for computing the rank is less efficient than calling NumPy's singular value decomposition. Here are timings for a random 100×100-matrix:

```
>>> A = np.random.uniform(0, 1, (100, 100))
>>> %timeit U, s, V = np.linalg.svd(A)
100 loops, best of 3: 3.7 ms per loop
>>> %timeit A, rank = Gaussian_elimination(A)
100 loops, best of 3: 22.3 ms per loop
```

5.9.10 Symbolic Linear Algebra

SymPy supports symbolic computations also for linear algebra operations. We may create a matrix and find its inverse and determinant:

```
>>> import sympy as sym
>>> A = sym.Matrix([[2, 0], [0, 5]])

>>> A**-1    # the inverse
Matrix([
[1/2,   0],
[  0, 1/5]])

>>> A.inv()  # the inverse
Matrix([
[1/2,   0],
[  0, 1/5]])

>>> A.det()  # the determinant
10
```

Note that the entries in the inverse matrix are rational numbers (`sym.Rational` objects to be precise).

Eigenvalues can also be computed exactly:

```
>>> A.eigenvals()
{2: 1, 5: 1}
```

The output is a dictionary meaning here that 2 is an eigenvalue with multiplicity 1 and 5 is an eigenvalue with multiplicity 1. It is more convenient to have the eigenvalues in a list:

```
>>> e = list(A.eigenvals().keys())
>>> e
[2, 5]
```

Eigenvector computations have a somewhat complicated output:

```
>>> A.eigenvects()
[(2, 1, [Matrix([
[1],
[0]])]), (5, 1, [Matrix([
[0],
[1]])])]
```

The output is a list of three-tuples, one for each eigenvalue and eigenvector. The three-tuple contains the eigenvalue, its multiplicity, and the eigenvector as a `sym.Matrix` object. To isolate the first eigenvector, we can index the list and tuple:

```
>>> v1 = A.eigenvects()[0][2]
>>> v1
Matrix([
[1],
[0]])
```

The vector is a `sym.Matrix` object with two indices. To extract the vector elements in a plain list, we can do this:

```
>>> v1 = [v1[i,0] for i in range(v1.shape[0])]
>>> v1
[1, 0]
```

The following code extracts all eigenvectors as a list of 2-lists, which may be a convenient data structure for the eigenvectors:

```
>>> v = [[t[2][0][i,0] for i in range(t[2][0].shape[0])]
         for t in A.eigenvects()]
>>> v
[[1, 0], [0, 1]]
```

The norm of a matrix or vector is an exact expression:

```
>>> A.norm()
sqrt(29)
>>> a = sym.Matrix([1, 2])   # vector [1, 2]
>>> a
```

```
Matrix([
[1],
[2]])
>>> a.norm()
sqrt(5)
```

The matrix-vector product and the dot product between vectors are done like this:

```
>>> A*a                      # matrix*vector
Matrix([
[ 2],
[10]])
>>> b = sym.Matrix([2, -1])  # vector [2, -1]
>>> a.dot(b)
0
```

Solving linear systems exactly is also possible:

```
>>> x = sym.Matrix([-1, 1])/2
>>> x
Matrix([
[-1/2],
[ 1/2]])
>>> b = A*x
>>> x = A.LUsolve(b)  # does it compute x?
>>> x                 # x is a matrix object
Matrix([
[-1/2],
[ 1/2]])
```

Sometimes one wants to convert `x` to a plain `numpy` array with `float` values:

```
>>> x = np.array([float(x[i,0].evalf())
                  for i in range(x.shape[0])])
>>> x
array([-0.5,  0.5])
```

Exact row operations can be done as exemplified here:

```
>>> A[1,:] + 2*A[0,:]  # [0,5] + 2*[2,0]
Matrix([[4, 5]])
```

We refer to the online SymPy linear algebra tutorial[7] for more information.

[7] http://docs.sympy.org/dev/tutorial/matrices.html

5.10 Plotting of Scalar and Vector Fields

Visualization of scalar and vector fields in Python is commonly done using Matplotlib or Mayavi. Both packages support basic visualization of 2D scalar and vector fields, but Mayavi offers more advanced three-dimensional visualization techniques, especially for 3D scalar and vector fields.

One can also use SciTools for visualizing 2D scalar and vector fields, using either Matplotlib, Gnuplot, or VTK as plotting engines, but this topic is omitted from the present book. However, for fast visualization of large 2D scalar fields, Gnuplot is a viable tool, and the SciTools interface offers a convenient MATLAB-style set of commands to operate Gnuplot.

To exemplify visualization of scalar and vector fields with Matplotlib and Mayavi, we use a common set of examples. A scalar function of x and y is visualized either as a flat two-dimensional plot with contour lines of the field, or as a three-dimensional surface where the height of the surface corresponds to the function value of the field. In the latter case we also add a three-dimensional parameterized curve to the plot.

To illustrate plotting of vector fields, we simply plot the gradient of the scalar field, together with the scalar field. Our convention for variable names goes as follows:

- `x`, `y` for one-dimensional coordinates along each axis direction.
- `xv`, `yv` for the corresponding vectorized coordinates in a 2D.
- `u`, `v` for the components of a vector field at points corresponding to `xv`, `yv`.

The following sections contain more mathematical details on the various scalar and vector fields we aim to plot.

5.10.1 Installation

Previously in the book we have explained how to obtain Matplotlib for various platforms. To obtain Mayavi on Ubuntu platforms you can write

Terminal

```
pip install mayavi --upgrade
```

For Mac OS X and Windows, we recommend using Anaconda. To obtain Mayavi for Anaconda you can write

Terminal

```
conda install mayavi
```

5.10.2 Surface Plots

We consider the 2D scalar field defined by

$$h(x, y) = \frac{h_0}{1 + \frac{x^2+y^2}{R^2}}. \tag{5.13}$$

$h(x, y)$ may model the height of an isolated circular mountain, h being the height above sea level, while x and y are Cartesian coordinates on the earth's surface, h_0 the height of the mountain, and R the radius of the mountain. Since mountains are actually quite flat (or more precisely, their heights are small compared to the horizontal extent), we use meter as length unit for vertical distances (z direction) and km as length unit for horizontal distances (x and y coordinates). Prior to all code below we have initialized h_0 and R with the following values: $h_0 = 2277$ m and $R = 4$ km.

Grid for 2D scalar fields Before we can plot $h(x, y)$, we need to create a rectangular grid in the xy plane with all the points used for plotting. Regardless of which plotting package we will use later on, the grid can be made as follows:

```
x = y = np.linspace(-10., 10., 41)
xv, yv = np.meshgrid(x, y, indexing='ij', sparse=False)

hv = h0/(1 + (xv**2+yv**2)/(R**2))
```

The grid is based on equally spaced coordinates `x` and `y` in the interval $[-10, 10]$ km. Note the mysterious extra parameters to `meshgrid` here, which are needed in order for the coordinates to have the right order such that the arithmetics in the expression for `hv` becomes correct. The expression computes the surface value at the 41×41 grid points in one vectorized operation.

A surface plot of a 2D scalar field $h(x, y)$ is a visualization of the surface $z = h(x, y)$ in three-dimensional space. Most plotting packages have functions which can be used to create surface plots of 2D scalar fields. These can be either *wireframe plots*, where only lines connecting the grid points are drawn, or plots where the faces of the surface are colored. In Fig. 5.12 we have shown two such plots of the surface $h(x, y)$. Section 5.11.1 presents the code which generates these plots.

5.10.3 Parameterized Curve

To illustrate the plotting of three-dimensional parameterized curves, we consider a trajectory that represents a circular climb to the top of the mountain:

$$\boldsymbol{r}(t) = \left(10\left(1 - \frac{t}{2\pi}\right)\cos(t)\right)\boldsymbol{i} + \left(10\left(1 - \frac{t}{2\pi}\right)\sin(t)\right)\boldsymbol{j} + \frac{h_0}{1 + \frac{100(1-t/(2\pi))^2}{R^2}}\boldsymbol{k}. \tag{5.14}$$

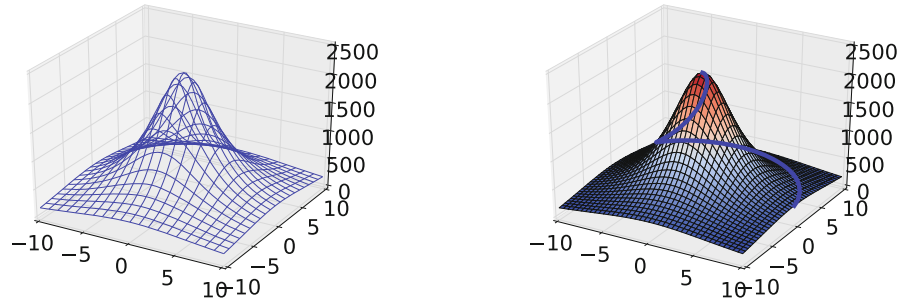


Fig. 5.12 Two different plots of a mountain. The right plot also shows a trajectory to the top of the mountain

Here $\boldsymbol{i}$, $\boldsymbol{j}$, and $\boldsymbol{k}$ denote the unit vectors in the x-, y-, and z-directions, respectively. The coordinates of $\boldsymbol{r}(t)$ can be produced by

```
s = np.linspace(0, 2*np.pi, 100)
curve_x = 10*(1 - s/(2*np.pi))*np.cos(s)
curve_y = 10*(1 - s/(2*np.pi))*np.sin(s)
curve_z = h0/(1 + 100*(1 - s/(2*np.pi))**2/(R**2))
```

The parameterized curve is shown together with the surface $h(x, y)$ in the right plot in Fig. 5.12.

5.10.4 Contour Lines

Contour lines are lines defined by the implicit equation $h(x, y) = C$, where C is some constant representing the contour level. Normally, we let C run over some equally spaced values, and very often, the plotting program computes the C values. To distinguish contours, one often associates each contour level C with its own color.

Figure 5.13 shows different ways contour lines can be used to visualize the surface $h(x, y)$. The first and last plot are visualizations utilizing two spatial dimensions. The first draws a small set of contour lines only, while the last one displays the surface as an image, whose colors reflect the values of the field, or equivalently, the height of the surface. The third plot actually combines three different types of contours, each type corresponding to keeping a coordinate constant and projecting the contours on a "wall". The code used to generate these plots is presented in Sect. 5.11.2.

5.10.5 The Gradient Vector Field

The *gradient vector field* ∇h of a 2D scalar field $h(x, y)$ is defined by

$$\nabla h = \frac{\partial h}{\partial x}\boldsymbol{i} + \frac{\partial h}{\partial y}\boldsymbol{j}. \tag{5.15}$$

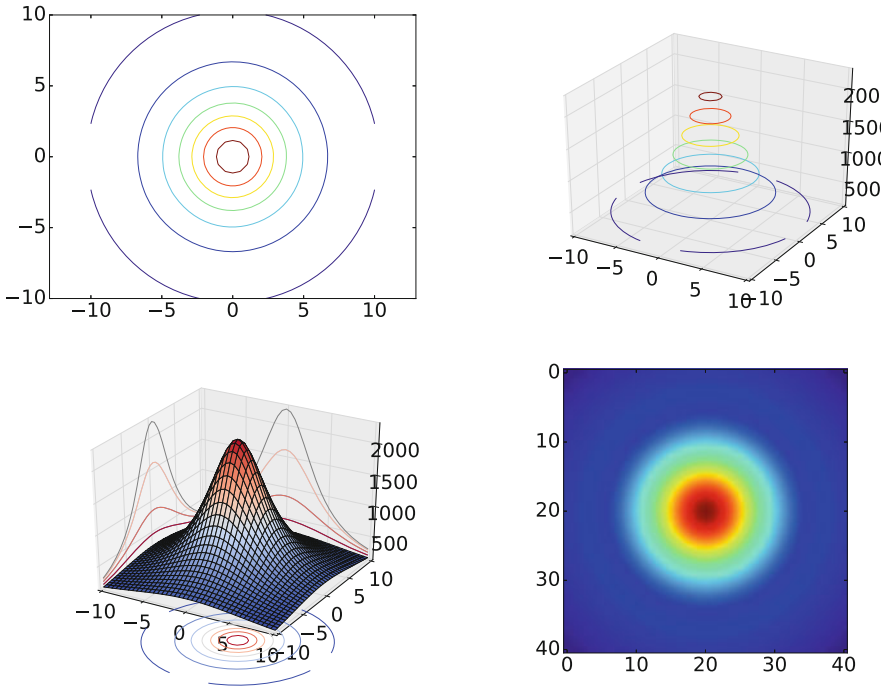


Fig. 5.13 Different types of contour plots of a 2D scalar field in two and three dimensions

One learns in vector calculus that the gradient points in the direction where h increases most, and that the gradients are orthogonal to the contour lines. This is something we can easily illustrate by creating 2D plots of the contours and the gradient field. A challenge in making such plots is to get the right arrow lengths so that the arrows are well visible, but they do not collide and make a cluttered visual impression. Since the arrows are drawn at each point in a 2D grid, one way of controlling the number of arrows is to control the resolution of the grid.

So, let us create a grid with 20 instead of 40 intervals in the horizontal directions:

```
x2 = y2 = np.linspace(-10.,10.,11)
x2v, y2v = np.meshgrid(x2, y2, indexing='ij', sparse=False)
h2v = h0/(1 + (x2v**2 + y2v**2)/(R**2)) # h on coarse grid
```

The gradient vector field of $h(x, y)$ can now be computed using the function `np.gradient`:

```
dhdx, dhdy = np.gradient(h2v) # dh/dx, dh/dy
```

The gradient field (5.15) together with the contours appear in Fig. 5.14, from which the orthogonality can be easily seen. Section 5.11.3 explains the code needed to make this plot.

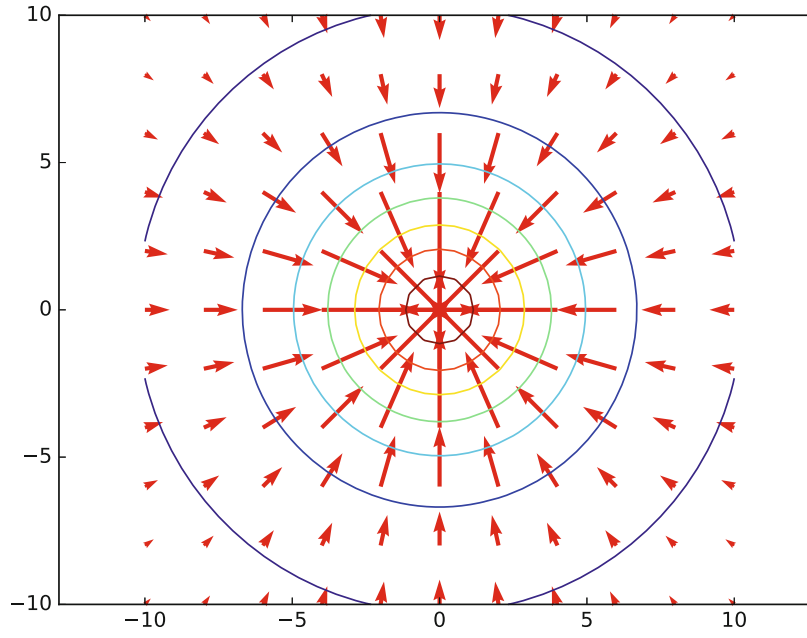


Fig. 5.14 Gradient field with contour plot

5.11 Matplotlib

We import any visualization package under the name `plt`, so for Matplotlib the import is done by

```
import matplotlib.pyplot as plt
```

When creating two-dimensional plots of scalar and vector fields, we shall make use of a Matplotlib `Axes` object, named `ax` and made by

```
fig = plt.figure(1)   # Get current figure
ax = fig.gca()        # Get current axes
```

For three-dimensional visualization, we need the following alternative lines:

```
from mpl_toolkits.mplot3d import Axes3D

fig = plt.figure(1)
ax = fig.gca(projection='3d')
```

5.11.1 Surface Plots

The Matplotlib functions for producing surface plots of 2D scalar fields are `ax.plot_wireframe` and `ax.plot_surface`. The first one produces a wire-

frame plot, and the second one colors the surface. The following code uses the functions to produce the plots shown in Fig. 5.12, once the grid has been defined as in Sect. 5.10.2, and the coordinates of the parameterized curve have been computed as in Sect. 5.10.3.

```
fig = plt.figure(1)
ax = fig.gca(projection='3d')
ax.plot_wireframe(xv, yv, hv, rstride=2, cstride=2)

# Simple plot of mountain and parametric curve
fig = plt.figure(2)
ax = fig.gca(projection='3d')
from matplotlib import cm
ax.plot_surface(xv, yv, hv, cmap=cm.coolwarm,
                rstride=1, cstride=1)

# add the parametric curve. linewidth controls the width of the curve
ax.plot(curve_x, curve_y, curve_z, linewidth=5)
```

Recall that a final `plt.show()` command is necessary to force Matplotlib to show a plot on the screen.

Note that the second plot in this figure is drawn using a finer grid. This is controlled with the `rstride` and `cstride` parameters, which sets the number of grid lines in each direction. Setting one of these to 1 means that a grid line is drawn for every value in the grid in the corresponding direction, and setting to 2 means that a grid line will be drawn for every two values in the grid. You will normally need to experiment with such parameters to get a visually attractive plot.

A surface with colors reflecting the height of the surface needs specification of a *color map*, which is a mapping between function values and colors. Above we applied the common `coolwarm` scheme which goes from blue ("cool" color for minimum values) to red ("warm" color for maximum values). There are lots of colormaps to choose from, and you have to experiment to find appropriate choices according to your taste and to the problem at hand.

To the latter plot we also added the parameterized curve $\boldsymbol{r}(t)$, defined by (5.14), using the command `plot`. The attribute `linewidth` is increased here in order to make the curve thicker and more visible. By default, Matplotlib adds plots to each other without any need for `plt.hold('on')`, although such a command can indeed be used.

5.11.2 Contour Plots

The following code exemplifies different types of contour plots. The first two plots (default two-dimensional and three-dimensional contour plots) are shown in Fig. 5.13. The next four plots appear in Fig. 5.15. Note that, when we asked Matplotlib to plot 10 contours, the response was, surprisingly, 9 contour lines, where one of the contours was incomplete. This kind of behavior may also be found in other plotting packages (such as MATLAB): the package will do its best to plot the requested number of complete contour lines, but there is no guarantee that this number is achieved exactly.

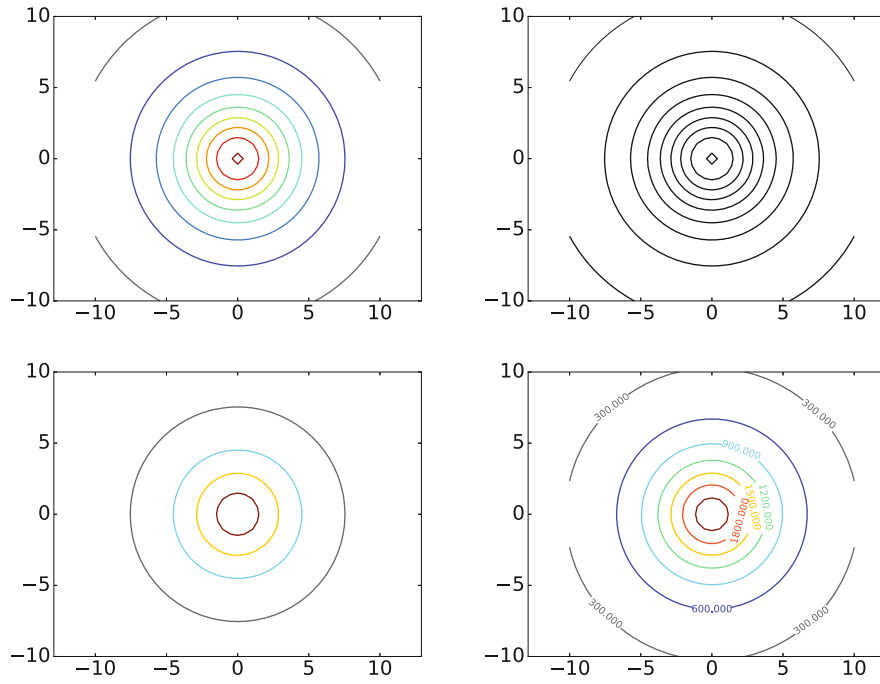


Fig. 5.15 Some other contour plots with Matplotlib: 10 contour lines (*upper left*), 10 black contour lines (*upper right*), specified contour levels (*lower left*), and labeled levels (*lower right*)

```
# Default two-dimensional contour plot with 7 colored lines
fig = plt.figure(3)
ax = fig.gca()
ax.contour(xv, yv, hv)
plt.axis('equal')

# Default three-dimensional contour plot
fig = plt.figure(4)
ax = fig.gca(projection='3d')
ax.contour(xv, yv, hv)

# Plot of mountain and contour lines projected on the
# coordinate planes
fig = plt.figure(5)
ax = fig.gca(projection='3d')
ax.plot_surface(xv, yv, hv, cmap=cm.coolwarm,
                rstride=1, cstride=1)
# zdir is the projection axis
# offset is the offset of the projection plane
ax.contour(xv, yv, hv, zdir='z', offset=-1000, cmap=cm.coolwarm)
ax.contour(xv, yv, hv, zdir='x', offset=-10,   cmap=cm.coolwarm)
ax.contour(xv, yv, hv, zdir='y', offset=10,    cmap=cm.coolwarm)

# View the contours by displaying as an image
fig = plt.figure(6)
ax = fig.gca()
ax.imshow(hv)
```

```
# 10 contour lines (equally spaced contour levels)
fig = plt.figure(7)
ax = fig.gca()
ax.contour(xv, yv, hv, 10)
plt.axis('equal')

# 10 black ('k') contour lines
fig = plt.figure(8)
ax = fig.gca()
ax.contour(xv, yv, hv, 10, colors='k')
plt.axis('equal')

# Specify the contour levels explicitly as a list
fig = plt.figure(9)
ax = fig.gca()
levels = [500., 1000., 1500., 2000.]
ax.contour(xv, yv, hv, levels=levels)
plt.axis('equal')

# Add labels with the contour level for each contour line
fig = plt.figure(10)
ax = fig.gca()
cs = ax.contour(xv, yv, hv)
plt.clabel(cs)
plt.axis('equal')
```

5.11.3 Vector Field Plots

The code for plotting the gradient field (5.15) together with contours goes as explained below, once the grid has been defined as in Sect. 5.10.5. The corresponding plot is shown in Fig. 5.14.

```
fig = plt.figure(11)
ax = fig.gca()
ax.quiver(x2v, y2v, dhdx, dhdy, color='r',
          angles='xy', scale_units='xy')
ax.contour(xv, yv, hv)
plt.axis('equal')
```

5.12 Mayavi

Mayavi is an advanced, free, easy to use, scientific data visualizer, with an emphasis on three-dimensional visualization techniques. The package is written in Python, and uses the Visualization Toolkit (VTK) in C++ for rendering graphics. Since VTK can be configured with different backends, so can Mayavi. Mayavi is cross platform and runs on most platforms, including Mac OS X, Windows, and Linux.

The web page http://docs.enthought.com/mayavi/mayavi/ collects pointers to all relevant documentation of Mayavi. We shall primarily deal with the `mayavi.mlab` module, which provides a simple interface to plotting of 2D scalar and vector fields with commands that mimic those of MATLAB. Let us import this module under our usual name `plt` for a plotting package:

```
import mayavi.mlab as plt
```

The official documentation of the `mlab` module is provided in two places, one for the basic functionality[8] and one for further functionality[9]. Basic figure handling[10] is very similar to the one we know from Matplotlib. Just as for Matplotlib, all plotting commands you do in `mlab` will go into the same figure, until you manually change to a new figure.

5.12.1 Surface Plots

Mayavi has the functions `mesh` and `surf` for producing surface plots. These are similar, but `surf` assumes an orthogonal grid, and uses this assumption to make efficient data structures, while `mesh` makes no such assumptions on the grid. Here we only use orthogonal grids and hence apply `surf`. The following code plots the surface $h(x, y)$ in (5.13), as well as the parameterized curve $\boldsymbol{r}(t)$ in (5.14). The resulting graphics appears in Fig. 5.16.

```
# Create a figure with white background and black foreground
plt.figure(1, fgcolor=(.0, .0, .0), bgcolor=(1.0, 1.0, 1.0))
# 'representation' sets type of plot, here a wireframe plot
plt.surf(xv, yv, hv, extent=(0,1,0,1,0,1),
         representation='wireframe')
# Decorate axes (nb_labels is the number of labels used
# in each direction)
plt.axes(xlabel='x', ylabel='y', zlabel='z', nb_labels=5,
         color=(0., 0., 0.))
# Decorate the plot with a title
plt.title('h(x,y)', size=0.4)

# Simple plot of mountain and parametric curve.
plt.figure(2, fgcolor=(.0, .0, .0), bgcolor=(1.0, 1.0, 1.0))
# Here, representation has default: colored surface elements
plt.surf(xv, yv, hv, extent=(0,1,0,1,0,1))
# Add the parametric curve. tube_radius is the width of the
# curve (use 'extent' for auto-scaling)
plt.plot3d(curve_x, curve_y, curve_z, tube_radius=0.2,
           extent=(0,1,0,1,0,1))

plt.figure(3, fgcolor=(.0, .0, .0), bgcolor=(1.0, 1.0, 1.0))
# Use 'warp_scale' for vertical scaling
plt.surf(xv, yv, hv, warp_scale=0.01, color=(.5, .5, .5))
plt.plot3d(curve_x, curve_y, 0.01*curve_z, tube_radius=0.2)
```

`surf` can produce wireframe plots, as well as plots where the faces of the surface are colored. The parameter `representation` controls this, as exemplified in the first two plots. The first plot was also decorated with axes and a title.

The calls to `plt.figure()` take three parameters: First the usual index for the plot, then two tuples of numbers , representing the RGB-values to be used for the foreground (`fgcolor`) and the background (`bgcolor`). White and black are (1,1,1)

[8] http://docs.enthought.com/mayavi/mayavi/auto/mlab_helper_functions.html
[9] http://docs.enthought.com/mayavi/mayavi/auto/mlab_other_functions.html
[10] http://docs.enthought.com/mayavi/mayavi/auto/mlab_figure.html

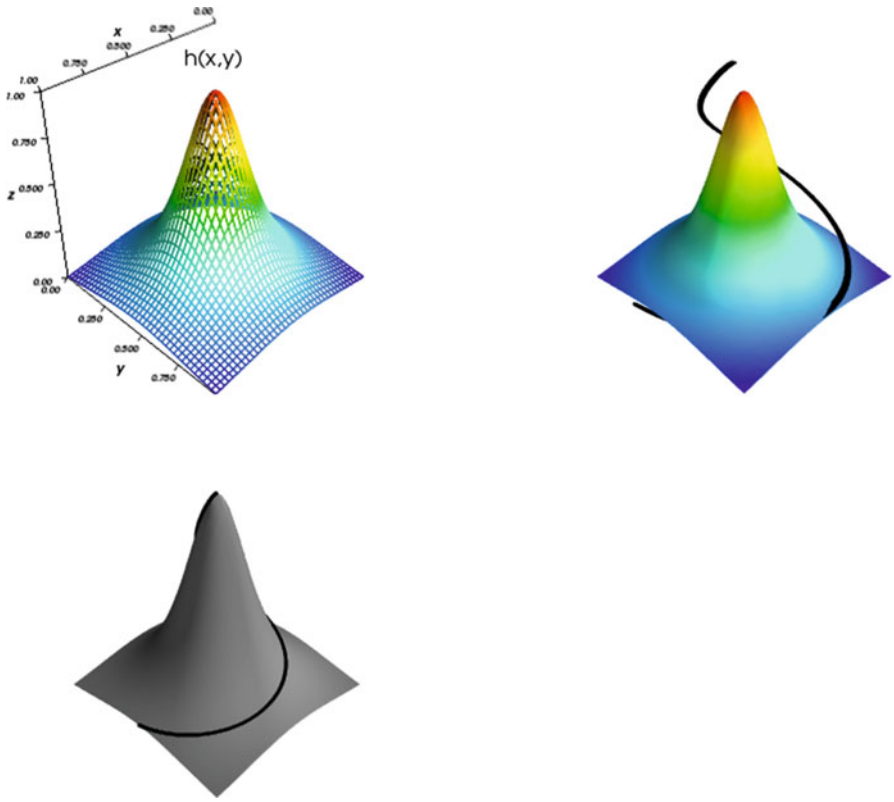


Fig. 5.16 Surface plots produced with the `surf` function of Mayavi: The curve $\boldsymbol{r}(t)$ is also shown in the two last plots

and (0,0,0), respectively. The foreground color is used for text and labels included in the plot. The `color` attribute in `plt.surf` adjusts the surface so that it is colored with small variations from the provided base color, here `(.5, .5, .5)`.

The command `plot3d` is used to plot the curve $\boldsymbol{r}(t)$. We have here increased the attribute `tube_radius` to make the curve thicker and more visible.

Mayavi does no auto-scaling of the axes by default (contrary to Matplotlib), so if the magnitudes in the vertical and horizontal directions are very different, as they are for $h(x, y)$, the plots may be very concentrated in one direction. We therefore need to apply some auto-scaling procedure. In Fig. 5.16 two such procedures are exemplified. In the first two plots the parameter `extent` is used. It tells Mayavi to auto-scale the surface and curve to fit the contents described by the six listed values (we will return to what these values mean when we have a more illustrating example). Since the curve and the surface span different areas in space, we see that they are auto-scaled differently in the second plot, with the undesired effect that $\boldsymbol{r}(t)$ is not drawn on the surface. The last plot has avoided this problem by using the `warp_scale` parameter for scaling the vertical direction. Not all Mayavi functions accept this parameter. A remedy for this is to scale the z-coordinates manually, as here exemplified in the last `plot3d`-call. As is seen, the curve is

drawn correctly with respect to the surface in the last plot. In the following we will use the `warp_scale` parameter to avoid such auto-scaling problems.

Subplots The two plots in Fig. 5.16 were created as separate figures. One can also create them as subplots within one figure:

```
plt.figure(4, fgcolor=(.0, .0, .0), bgcolor=(1.0, 1.0, 1.0))
plt.mesh(xv, yv, hv, extent=(0, 0.25, 0, 0.25, 0, 0.25),
         colormap='cool')
plt.outline(plt.mesh(
    xv, yv, hv,
    extent=(0.375, 0.625, 0, 0.25, 0, 0.25),
    colormap='Accent'))
plt.outline(plt.mesh(
    xv, yv, hv, extent=(0.75, 1, 0, 0.25, 0, 0.25),
    colormap='prism'), color=(.5, .5, .5))
```

The result is shown in Fig. 5.17. Three separate `mesh` commands are run, each producing a new plot in the current figure. The commands use different values for the `colormap` attribute to color the surface in different ways. When this attribute is not provided, as in the code producing the two first plots in Fig. 5.16, a default colormap is used.

The `plt.outline` command is used to create a frame around the subplots, and as seen, we exemplify this possibility for the last two subplots, but not the first one. We see that one of the two frames has a different color, obtained by setting the `color` attribute of the `plt.outline` command.

From the computer code it is hopefully clear that the six values listed in `extent` represent fractions of the cube `(0,1,0,1,0,1)`, where the corresponding plots are placed. The extents for the three plots are here defined such that they do not overlap.

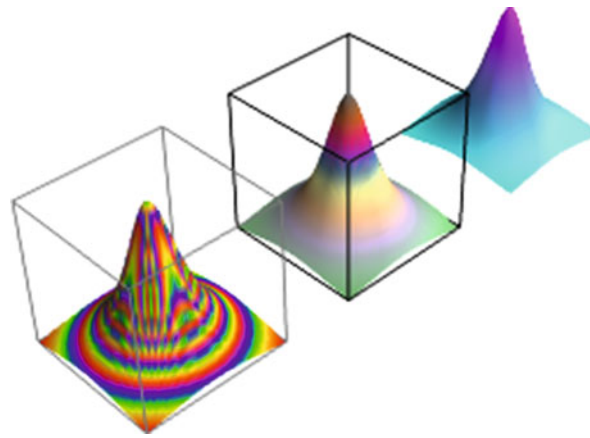


Fig. 5.17 A plot with three subplots created with Mayavi

5.12.2 Contour Plots

The following code exemplifies how one can produce contour plots with Mayavi. The code is very similar to that of Matplotlib, but one difference is that the attribute `contours` now can represent the number of levels, as well as the levels themselves. The plots are shown in Fig. 5.18.

```
# Default contour plot plotted together with surf.
plt.figure(5, fgcolor=(.0, .0, .0), bgcolor=(1.0, 1.0, 1.0))
plt.surf(xv, yv, hv, warp_scale=0.01)
plt.contour_surf(xv, yv, hv, warp_scale=0.01)

# 10 contour lines (equally spaced contour levels).
plt.figure(6, fgcolor=(.0, .0, .0), bgcolor=(1.0, 1.0, 1.0))
plt.contour_surf(xv, yv, hv, contours=10, warp_scale=0.01)

# 10 contour lines (equally spaced contour levels) together
# with surf. Black color for contour lines.
plt.figure(7, fgcolor=(.0, .0, .0), bgcolor=(1.0, 1.0, 1.0))
plt.surf(xv, yv, hv, warp_scale=0.01)
plt.contour_surf(xv, yv, hv, contours=10, color=(0., 0., 0.),
                 warp_scale=0.01)

# Specify the contour levels explicitly as a list.
plt.figure(8, fgcolor=(.0, .0, .0), bgcolor=(1.0, 1.0, 1.0))
levels = [500., 1000., 1500., 2000.]
plt.contour_surf(xv, yv, hv, contours=levels, warp_scale=0.01)

# View the contours by displaying as an image.
plt.figure(9, fgcolor=(.0, .0, .0), bgcolor=(1.0, 1.0, 1.0))
plt.imshow(hv)
```

Note that there is no function in Mayavi which labels the contours.

Contour plots in Mayavi are shown in three-dimensional space, but you can rotate and look at them from above if you want a two-dimensional plot. Their visual appearance may be enhanced by also including the surface plot itself. We have done this for the top and middle left plots in Fig. 5.18. There is a clear difference in visual impression between these two plots: in the first one, default surface- and contour coloring is used, resulting in less visible contours, but in the middle left plot (`plt.figure` 6), we set black contours to make them better stand out.

5.12.3 Vector Field Plots

Mayavi supports only vector fields in three-dimensional space. We will therefore visualize the two-dimensional gradient field (5.15) by adding a third component of zero. The following code plots this gradient field together with the contours of h.

```
plt.figure(11, fgcolor=(.0, .0, .0), bgcolor=(1.0, 1.0, 1.0))
plt.contour_surf(xv, yv, hv, contours=20, warp_scale=0.01)
```

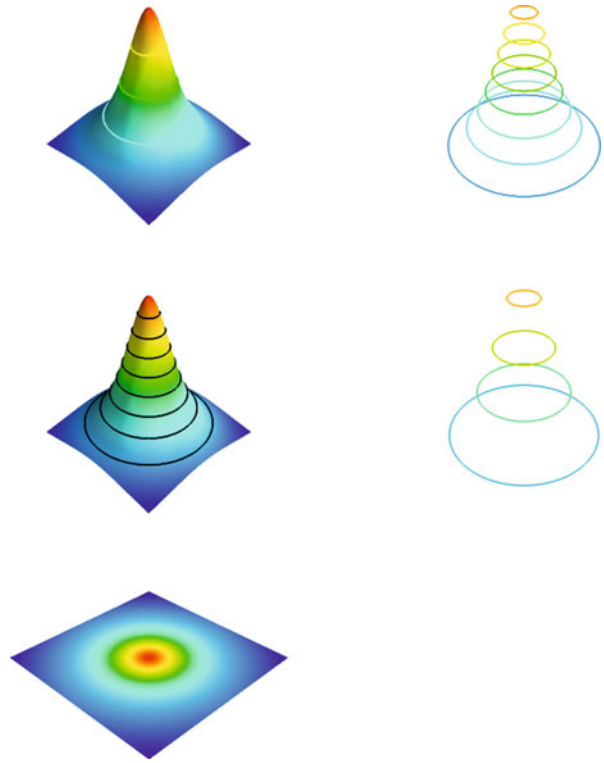


Fig. 5.18 Some contour plots with Mayavi

```
# mode controls the style how vectors are drawn
# color controls the colors of the vectors
# scale_mode='none' ensures that vectors are drawn with the same length
plt.quiver3d(x2v, y2v, 0.01*h2v, dhdx, dhdy, np.zeros_like(dhdx),
             mode='arrow', color=(1,0,0), scale_mode='none')
```

This will produce a 3D view, which we again can rotate to obtain a 2D view. The result is shown in Fig. 5.19, which is similar to Fig. 5.14.

5.12.4 A 3D Scalar Field and Its Gradient Field

Mayavi has functionality for drawing contour surfaces of 3D scalar fields. Let us consider the 3D scalar field

$$g(x, y, z) = z - h(x, y). \tag{5.16}$$

A three-dimensional grid for g can be computed as follows.

```
x = y = np.linspace(-10.,10.,41)
z = np.linspace(0, 50, 41)
```

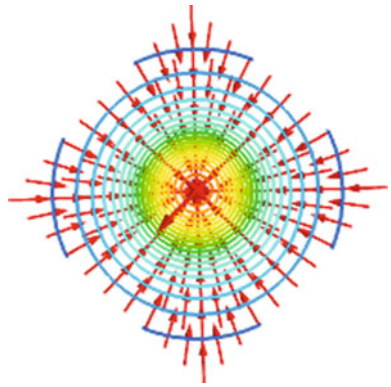


Fig. 5.19 Gradient field with contour plot

```
xv, yv, zv = np.meshgrid(x, y, z,
                         sparse=False, indexing='ij')
hv = 0.01*h0/(1 + (xv**2+yv**2)/(R**2))
gv = zv - hv
```

The contours are now surfaces defined by the implicit equation $g(x, y, z) = C$, corresponding to vertical shifts of the surface $h(x, y)$.

A corresponding vector field can be calculated:

$$\nabla g = \frac{\partial g}{\partial x}\boldsymbol{i} + \frac{\partial g}{\partial y}\boldsymbol{j} + \frac{\partial g}{\partial z}\boldsymbol{k}. \tag{5.17}$$

numpy's gradient function can be used to compute a gradient vector field in 3D as well, but you need a three-dimensional grid for the field as input. For the field (5.16), the gradient field is computed as follows.

```
x2 = y2 = np.linspace(-10.,10.,5)
z2 = np.linspace(0, 50, 5)
x2v, y2v, z2v = np.meshgrid(x2, y2, z2,
                            indexing='ij', sparse=False)
h2v = 0.01*h0/(1 + (x2v**2 + y2v**2)/(R**2))
g2v = z2v - h2v
dhdx, dhdy, dhdz = np.gradient(g2v)
```

Again we have used a coarser grid for the vector field.

To visualize the field (5.16) and its gradient field together, we draw enough contours, as we did in the 2D case in Fig. 5.14. The following code can be used.

```
plt.figure(12, fgcolor=(.0, .0, .0), bgcolor=(1.0, 1.0, 1.0))
# opacity controls how contours are visible through each other
plt.contour3d(xv, yv, zv, gv, contours=7, opacity=0.5)
# scale_mode='none': vectors should not be scaled
plt.quiver3d(x2v, y2v, z2v, dhdx, dhdy, dhdz, mode='arrow',
             scale_mode='none', opacity=0.5)
```

The result is shown in Fig. 5.20.

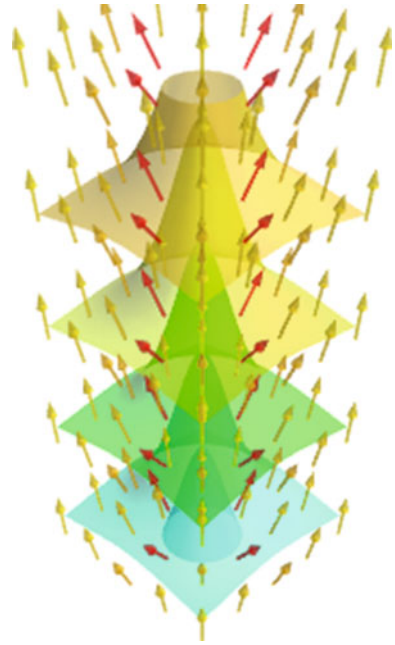


Fig. 5.20 The 3D scalar field (5.16) and its gradient field

This example demonstrates some of the challenges in plotting three-dimensional vector fields. The vectors must not be too dense, and not too long. It is inevitable that contours shadow one another. Fortunately, Mayavi supports an opacity setting, which controls how contours are visible through each other. Visualizing a 3D scalar field is clearly challenging, and we have only touched the subject.

5.12.5 Animations

It is straightforward to create animations with Mayavi. In the following code the function $h(x, y)$ is scaled vertically, for different scaling constants between 0 and 1, and each plot is saved in its own file. The files can then be combined to a standard video file.

```
plt.figure(13, fgcolor=(.0, .0, .0), bgcolor=(1.0, 1.0, 1.0))
s = plt.surf(xv, yv, hv, warp_scale=0.01)

for i in range(10):
    # s.mlab_source.scalars is a handle for the values of the surface,
    # and is updated here
    s.mlab_source.scalars = hv*0.1*(i+1)
    plt.savefig('tmp_%04d.png' % i)
```

5.13 Summary

5.13.1 Chapter Topics

This chapter has introduced computing with arrays and plotting curve data stored in arrays. The Numerical Python package contains lots of functions for array computing, including the ones listed in the table below. Plotting has been done with tools that closely resemble the syntax of MATLAB.

Construction	Meaning
`array(ld)`	copy list data `ld` to a `numpy` array
`asarray(d)`	make array of data `d` (no data copy if already array)
`zeros(n)`	make a `float` vector/array of length `n`, with zeros
`zeros(n, int)`	make an `int` vector/array of length `n` with zeros
`zeros((m,n))`	make a two-dimensional `float` array with shape (`m`,`n`)
`zeros_like(x)`	make array of same shape and element type as `x`
`linspace(a,b,m)`	uniform sequence of `m` numbers in $[a, b]$
`a.shape`	tuple containing `a`'s shape
`a.size`	total no of elements in `a`
`len(a)`	length of a one-dim. array `a` (same as `a.shape[0]`)
`a.dtype`	the type of elements in `a`
`a.reshape(3,2)`	return `a` reshaped as 3×2 array
`a[i]`	vector indexing
`a[i,j]`	two-dim. array indexing
`a[1:k]`	slice: reference data with indices `1,2,...,k-1`
`a[1:10:3]`	slice: reference data with indices `1,4,7`
`b = a.copy()`	copy an array
`sin(a), exp(a), ...`	`numpy` functions applicable to arrays
`c = concatenate((a, b))`	`c` contains `a` with `b` appended
`c = where(cond, a1, a2)`	`c[i] = a1[i]` if `cond[i]`, else `c[i] = a2[i]`
`isinstance(a, ndarray)`	is `True` if `a` is an array

Array computing When we apply a Python function `f(x)` to a Numerical Python array `x`, the result is the same as if we apply `f` to each element in `x` separately. However, when `f` contains `if` statements, these are in general invalid if an array `x` enters the boolean expression. We then have to rewrite the function, often by applying the `where` function from Numerical Python.

Plotting curves Sections 5.3.1 and 5.3.2 provide a quick overview of how to plot curves with the aid of Matplotlib. The same examples coded with the Easyviz plotting interface appear in Sect. 5.3.3.

Making movies Each frame in a movie must be a hardcopy of a plot in PNG format. These plot files should have names containing a counter padded with leading zeros. One example may be `tmp_0000.png`, `tmp_0001.png`, `tmp_0002.png`.

Having the plot files with names on this form, we can make an animated GIF movie in the file `movie.gif`, with two frames per second, by

```
os.system('convert -delay 50 tmp_*.png movie.gif')
```

Alternatively, we may combine the plot files to a Flash video:

```
os.system('ffmpeg -r 5 -i tmp_%04d.png -vcodec flv movie.flv')
```

Other formats can be made using other codecs, see Sect. 5.3.5.

Terminology The important topics in this chapter are

- array computing
- vectorization
- plotting
- animations

5.13.2 Example: Animating a Function

Problem In this chapter's summarizing example we shall visualize how the temperature varies downward in the earth as the surface temperature oscillates between high day and low night values. One question may be: What is the temperature change 10 m down in the ground if the surface temperature varies between 2 C in the night and 15 C in the day?

Let the z axis point downwards, towards the center of the earth, and let $z = 0$ correspond to the earth's surface. The temperature at some depth z in the ground at time t is denoted by $T(z,t)$. If the surface temperature has a periodic variation around some mean value T_0, according to

$$T(0,t) = T_0 + A\cos(\omega t),$$

one can find, from a mathematical model for heat conduction, that the temperature at an arbitrary depth is

$$T(z,t) = T_0 + Ae^{-az}\cos(\omega t - az), \quad a = \sqrt{\frac{\omega}{2k}}. \tag{5.18}$$

The parameter k reflects the ground's ability to conduct heat (k is called the *thermal diffusivity* or the *heat conduction coefficient*).

The task is to make an animation of how the temperature profile in the ground, i.e., T as a function of z, varies in time. Let ω correspond to a time period of 24 hours. The mean temperature T_0 is taken as 10 C, and the maximum variation A is assumed to be 10 C. The heat conduction coefficient k may be set as 1 mm^2/s (which is 10^{-6} m^2/s in proper SI units).

Solution To animate $T(z,t)$ in time, we need to make a loop over points in time, and in each pass in the loop we must save a plot of T, as a function of z, to file. The plot files can then be combined to a movie. The algorithm becomes

- for $t_i = i\Delta t$, $i = 0, 1, 2 \ldots, n$:
  - plot the curve $y(z) = T(z, t_i)$
  - store the plot in a file
- combine all the plot files into a movie

It can be wise to make a general `animate` function where we just feed in some $f(x,t)$ function and make all the plot files. If `animate` has arguments for setting the labels on the axis and the extent of the y axis, we can easily use `animate` also for a function $T(z,t)$ (we just use z as the name for the x axis and T as the name for the y axis in the plot). Recall that it is important to fix the extent of the y axis in a plot when we make animations, otherwise most plotting programs will automatically fit the extent of the axis to the current data, and the tick marks on the y axis will jump up and down during the movie. The result is a wrong visual impression of the function.

The names of the plot files must have a common stem appended with some frame number, and the frame number should have a fixed number of digits, such as 0001, 0002, etc. (if not, the sequence of the plot files will not be correct when we specify the collection of files with an asterisk for the frame numbers, e.g., as in `tmp*.png`). We therefore include an argument to `animate` for setting the name stem of the plot files. By default, the stem is `tmp_`, resulting in the filenames `tmp_0000.png`, `tmp_0001.png`, `tmp_0002.png`, and so forth. Other convenient arguments for the `animate` function are the initial time in the plot, the time lag Δt between the plot frames, and the coordinates along the x axis. The `animate` function then takes the form

```
def animate(tmax, dt, x, function, ymin, ymax, t0=0,
            xlabel='x', ylabel='y', filename='tmp_'):
    t = t0
    counter = 0
    while t <= tmax:
        y = function(x, t)
        plot(x, y, '-',
             axis=[x[0], x[-1], ymin, ymax],
             title='time=%2d h' % (t/3600.0),
             xlabel=xlabel, ylabel=ylabel,
             savefig=filename + '%04d.png' % counter)
        savefig('tmp_%04d.pdf' % counter)
        t += dt
        counter += 1
```

The $T(z,t)$ function is easy to implement, but we need to decide whether the parameters A, ω, T_0, and k shall be arguments to the Python implementation of $T(z,t)$ or if they shall be global variables. Since the `animate` function expects that the function to be plotted has only two arguments, we must implement $T(z,t)$ as `T(z,t)` in Python and let the other parameters be global variables (Sects. 7.1.1 and 7.1.2 explain this problem in more detail and present a better implementation). The `T(z,t)` implementation then reads

```
def T(z, t):
    # T0, A, k, and omega are global variables
    a = sqrt(omega/(2*k))
    return T0 + A*exp(-a*z)*cos(omega*t - a*z)
```

Suppose we plot $T(z,t)$ at n points for $z \in [0, D]$. We make such plots for $t \in [0, t_{\max}]$ with a time lag Δt between the them. The frames in the movie are now made by

```
# set T0, A, k, omega, D, n, tmax, dt
z = linspace(0, D, n)
animate(tmax, dt, z, T, T0-A, T0+A, 0, 'z', 'T')
```

We have here set the extent of the y axis in the plot as $[T_0 - A, T_0 + A]$, which is in accordance with the $T(z,t)$ function.

The call to `animate` above creates a set of files with names of the form `tmp_*.png`. Out of these files we can create an animated GIF movie or a video in, e.g., Flash format by running operating systems commands with `convert` and `avconv` (or `ffmpeg`):

```
os.system('convert -delay 50 tmp_*.png movie.gif')
os.system('avconv -i tmp_%04d.png -r 5 -vcodec flv movie.flv')
```

See Sect. 5.3.5 for how to create videos in other formats.

It now remains to assign proper values to all the global variables in the program: `n`, `D`, `T0`, `A`, `omega`, `dt`, `tmax`, and `k`. The oscillation period is 24 hours, and ω is related to the period P of the cosine function by $\omega = 2\pi/P$ (realize that $\cos(t2\pi/P)$ has period P). We then express $P = 24$ h as $24 \cdot 60 \cdot 60$ s and compute ω as $2\pi/P \approx 7 \cdot 10^{-5}$ s^{-1}. The total simulation time can be 3 periods, i.e., $t_{\max} = 3P$. The $T(z,t)$ function decreases exponentially with the depth z so there is no point in having the maximum depth D larger than the depth where T is visually zero, say 0.001. We have that $e^{-aD} = 0.001$ when $D = -a^{-1} \ln 0.001$, so we can use this estimate in the program. The proper initialization of all parameters can then be expressed as follows:

```
k = 1E-6          # thermal diffusivity (in m*m/s)
P = 24*60*60.     # oscillation period of 24 h (in seconds)
omega = 2*pi/P
dt = P/24         # time lag: 1 h
tmax = 3*P        # 3 day/night simulation
T0 = 10           # mean surface temperature in Celsius
A = 10            # amplitude of the temperature variations in Celsius
a = sqrt(omega/(2*k))
D = -(1/a)*log(0.001) # max depth
n = 501           # no of points in the z direction
```

Note that it is very important to use consistent units. Here we express all units in terms of meter, second, and Kelvin or Celsius.

We encourage you to run the program `heatwave.py` to see the movie. The hardcopy of the movie is in the file `movie.gif`. Figure 5.21 displays two snapshots in time of the $T(z,t)$ function.

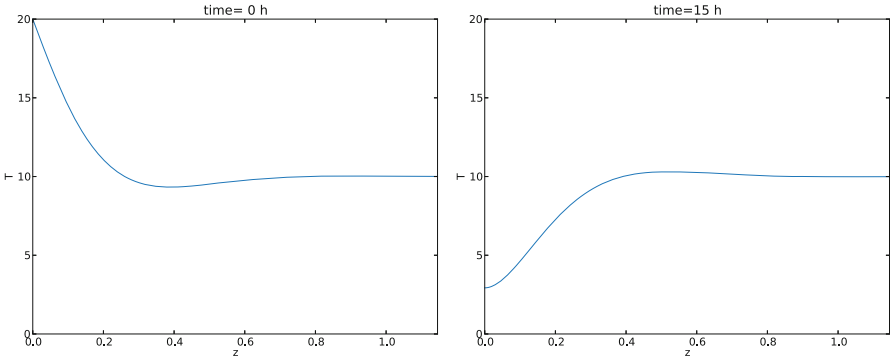


Fig. 5.21 Plot of the temperature $T(z,t)$ in the ground for two different t values

Scaling In this example, as in many other scientific problems, it was easier to write the code than to assign proper physical values to the input parameters in the program. To learn about the physical process, here how heat propagates from the surface and down in the ground, it is often advantageous to scale the variables in the problem so that we work with dimensionless variables. Through the scaling procedure we normally end up with much fewer physical parameters that must be assigned values. Let us show how we can take advantage of scaling the present problem.

Consider a variable x in a problem with some dimension. The idea of scaling is to introduce a new variable $\bar{x} = x/x_c$, where x_c is a *characteristic size* of x. Since x and x_c have the same dimension, the dimension cancels in $\bar{x}$ such that $\bar{x}$ is dimensionless. Choosing x_c to be the expected maximum value of x, ensures that $\bar{x} \leq 1$, which is usually considered a good idea. That is, we try to have all dimensionless variables varying between zero and one. For example, we can introduce a dimensionless z coordinate: $\bar{z} = z/D$, and now $\bar{z} \in [0,1]$. Doing a proper scaling of a problem is challenging so for now it is sufficient to just follow the steps below – and not worry why we choose a certain scaling.

In the present problem we introduce these dimensionless variables:

$$\bar{z} = z/D$$
$$\bar{T} = \frac{T - T_0}{A}$$
$$\bar{t} = \omega t$$

We now insert $z = \bar{z}D$ and $t = \bar{t}/\omega$ in the expression for $T(z,t)$ and get

$$T = T_0 + Ae^{-b\bar{z}}\cos(\bar{t} - b\bar{z}), \quad b = aD$$

or

$$\bar{T}(\bar{z},\bar{t}) = \frac{T - T_0}{A} = e^{-b\bar{z}}\cos(\bar{t} - b\bar{z})\,.$$

We see that $\bar{T}$ depends on only *one* dimensionless parameter b in addition to the independent dimensionless variables $\bar{z}$ and $\bar{t}$. It is common practice at this stage of the scaling to just drop the bars and write

$$T(z,t) = e^{-bz}\cos(t - bz)\,. \tag{5.19}$$

This function is much simpler to plot than the one with lots of physical parameters, because now we know that T varies between -1 and 1, t varies between 0 and 2π for one period, and z varies between 0 and 1. The scaled temperature has only one parameter b in addition to the independent variable. That is, the shape of the graph is completely determined by b.

In our previous movie example, we used specific values for D, ω, and k, which then implies a certain $b = D\sqrt{\omega/(2k)}$ (≈ 6.9). However, we can now run different b values and see the effect on the heat propagation. Different b values will in our problems imply different periods of the surface temperature variation and/or different heat conduction values in the ground's composition of rocks. Note that doubling ω and k leaves the same b – it is only the fraction ω/k that influences the value of b.

We can reuse the `animate` function also in the scaled case, but we need to make a new $T(z,t)$ function and, e.g., a main program where b can be read from the command line:

```
def T(z, t):
    return exp(-b*z)*cos(t - b*z)  # b is global

b = float(sys.argv[1])
n = 401
z = linspace(0, 1, n)
animate(3*2*pi, 0.05*2*pi, z, T, -1.2, 1.2, 0, 'z', 'T')
movie('tmp_*.png', encoder='convert', fps=2,
      output_file='tmp_heatwave.gif')
os.system('convert -delay 50 tmp_*.png movie.gif')
```

Running the program, found as the file `heatwave_scaled.py`, for different b values shows that b governs how deep the temperature variations on the surface $z = 0$ penetrate. A large b makes the temperature changes confined to a thin layer close to the surface, while a small b leads to temperature variations also deep down in the ground. You are encouraged to run the program with $b = 2$ and $b = 20$ to experience the major difference, or just view the ready-made animations[11].

We can understand the results from a physical perspective. Think of increasing ω, which means reducing the oscillation period so we get a more rapid temperature variation. To preserve the value of b we must increase k by the same factor. Since a large k means that heat quickly spreads down in the ground, and a small k implies the opposite, we see that more rapid variations at the surface requires a larger k to more quickly conduct the variations down in the ground. Similarly, slow temperature variations on the surface can penetrate deep in the ground even if the ground's ability to conduct (k) is low.

[11] http://hplgit.github.io/scipro-primer/video/heatwave.html

5.14 Exercises

Exercise 5.1: Fill lists with function values
Define

$$h(x) = \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}x^2}. \tag{5.20}$$

Fill lists `xlist` and `hlist` with x and $h(x)$ values for 41 uniformly spaced x coordinates in $[-4, 4]$.

Hint You may adapt the example in Sect. 5.2.1.
Filename: `fill_lists`.

Exercise 5.2: Fill arrays; loop version
The aim is to fill two arrays `x` and `y` with x and $h(x)$ values, respectively, where $h(x)$ is defined in (5.20). Let the x values be as in Exercise 5.1. Create empty `x` and `y` arrays and compute each element in `x` and `y` with a `for` loop.
Filename: `fill_arrays_loop`.

Exercise 5.3: Fill arrays; vectorized version
Vectorize the code in Exercise 5.2 by creating the x values using the `linspace` function from the `numpy` package and by evaluating $h(x)$ for an array argument.
Filename: `fill_arrays_vectorized`.

Exercise 5.4: Plot a function
Make a plot of the function in Exercise 5.1 for $x \in [-4, 4]$.
Filename: `plot_Gaussian`.

Exercise 5.5: Apply a function to a vector
Given a vector $v = (2, 3, -1)$ and a function $f(x) = x^3 + xe^x + 1$, apply f to each element in v. Then calculate by hand $f(v)$ as the NumPy expression `v**3 + v*exp(v) + 1` using vector computing rules. Demonstrate that the two results are equal.
Filename: `apply_vecfunc`.

Exercise 5.6: Simulate by hand a vectorized expression
Suppose `x` and `t` are two arrays of the same length, entering a vectorized expression

```
y = cos(sin(x)) + exp(1/t)
```

If `x` holds two elements, 0 and 2, and `t` holds the elements 1 and 1.5, calculate by hand (using a calculator) the `y` array. Thereafter, write a program that mimics the series of computations you did by hand (typically a sequence of operations of the kind we listed in Sect. 5.1.3 – use explicit loops, but at the end you can use Numerical Python functionality to check the results).
Filename: `simulate_vector_computing`.

Exercise 5.7: Demonstrate array slicing
Create an array `w` with values $0, 0.1, 0.2, \ldots, 3$. Write out `w[:]`, `w[:-2]`, `w[::5]`, `w[2:-2:6]`. Convince yourself in each case that you understand which elements of the array that are printed.
Filename: `slicing`.

Exercise 5.8: Replace list operations by array computing
The data analysis problem in Sect. 2.6.2 is solved by list operations. Convert the list to a two-dimensional array and perform the computations using array operations (i.e., no explicit loops, but you need a loop to make the printout).
Filename: `sun_data_vec`.

Exercise 5.9: Plot a formula
Make a plot of the function $y(t) = v_0 t - \frac{1}{2}gt^2$ for $v_0 = 10$, $g = 9.81$, and $t \in [0, 2v_0/g]$. Set the axes labels as `time (s)` and `height (m)`.
Filename: `plot_ball1`.

Exercise 5.10: Plot a formula for several parameters
Make a program that reads a set of v_0 values from the command line and plots the corresponding curves $y(t) = v_0 t - \frac{1}{2}gt^2$ in the same figure, with $t \in [0, 2v_0/g]$ for each curve. Set $g = 9.81$.

Hint You need a different vector of t coordinates for each curve.
Filename: `plot_ball2`.

Exercise 5.11: Specify the extent of the axes in a plot
Extend the program from Exercises 5.10 such that the minimum and maximum t and y values are computed, and use the extreme values to specify the extent of the axes. Add some space above the highest curve to make the plot look better.
Filename: `plot_ball3`.

Exercise 5.12: Plot exact and inexact Fahrenheit-Celsius conversion formulas
A simple rule to quickly compute the Celsius temperature from the Fahrenheit degrees is to subtract 30 and then divide by 2: $C = (F - 30)/2$. Compare this curve against the exact curve $C = (F - 32)5/9$ in a plot. Let F vary between -20 and 120.
Filename: `f2c_shortcut_plot`.

Exercise 5.13: Plot the trajectory of a ball
The formula for the trajectory of a ball is given by

$$f(x) = x \tan\theta - \frac{1}{2v_0^2}\frac{gx^2}{\cos^2\theta} + y_0, \tag{5.21}$$

where x is a coordinate along the ground, g is the acceleration of gravity, v_0 is the size of the initial velocity, which makes an angle θ with the x axis, and $(0, y_0)$ is the initial position of the ball.

In a program, first read the input data y_0, θ, and v_0 from the command line. Then plot the trajectory $y = f(x)$ for $y \geq 0$.
Filename: `plot_trajectory`.

Exercise 5.14: Plot data in a two-column file
The file `src/plot/xy.dat`[12] contains two columns of numbers, corresponding to x and y coordinates on a curve. The start of the file looks as this:

```
-1.0000       -0.0000
-0.9933       -0.0087
-0.9867       -0.0179
-0.9800       -0.0274
-0.9733       -0.0374
```

Make a program that reads the first column into a list `x` and the second column into a list `y`. Plot the curve. Print out the mean y value as well as the maximum and minimum y values.

Hint Read the file line by line, split each line into words, convert to `float`, and append to `x` and `y`. The computations with `y` are simpler if the list is converted to an array.
Filename: `read_2columns`.

Remarks The function `loadtxt` in `numpy` can read files with tabular data (any number of columns) and return the data in a two-dimensional array:

```
import numpy as np
# Read table of floats
data = np.loadtxt('xy.dat', dtype=np.float)
# Extract one-dim arrays from two-dim data
x = data[:,0]  # column with index 0
y = data[:,1]  # column with index 1
```

The present exercise asks you to implement a simplified version of `loadtxt`, but for later loading of a file with tabular data into an array you will certainly use `loadtxt`.

Exercise 5.15: Write function data to file
We want to dump x and $f(x)$ values to a file, where the x values appear in the first column and the $f(x)$ values appear in the second. Choose n equally spaced x values in the interval $[a, b]$. Provide f, a, b, n, and the filename as input data on the command line.

Hint You may use the `StringFunction` tool (see Sects. 4.3.3 and 5.5.1) to turn the textual expression for f into a Python function. (Note that the program from Exercise 5.14 can be used to read the file generated in the present exercise into arrays again for visualization of the curve $y = f(x)$.)
Filename: `write_cml_function`.

[12] http://tinyurl.com/pwyasaa/plot/xy.dat

Exercise 5.16: Plot data from a file
The files `density_water.dat` and `density_air.dat` files in the folder `src/plot`[13] contain data about the density of water and air (respectively) for different temperatures. The data files have some comment lines starting with # and some lines are blank. The rest of the lines contain density data: the temperature in the first column and the corresponding density in the second column. The goal of this exercise is to read the data in such a file and plot the density versus the temperature as distinct (small) circles for each data point. Let the program take the name of the data file as command-line argument. Apply the program to both files.
Filename: `read_density_data`.

Exercise 5.17: Write table to file
Given a function of two parameters x and y, we want to create a file with a table of function values. The left column of the table contains y values in decreasing order as we go down the rows, and the last row contains the x values in increasing order. That is, the first column and the last row act like numbers on an x and y axis in a coordinate system. The rest of the table cells contains function values corresponding to the x and y values for the respective rows and columns. For example, if the function formula is $x + 2y$, x runs from 0 to 2 in steps of 0.5, and y run from -1 to 2 in steps of 1, the table looks as follows:

```
    2    4  4.5    5  5.5    6
    1    2  2.5    3  3.5    4
    0    0  0.5    1  1.5    2
   -1   -2 -1.5   -1 -0.5    0

         0  0.5    1  1.5    2
```

The task is to write a function

```
def write_table_to_file(f, xmin, xmax, nx, ymin, ymax, ny,
                        width=10, decimals=None,
                        filename='table.dat'):
```

where `f` is the formula, given as a Python function; `xmin`, `xmax`, `ymin`, and `ymax` are the minimum and maximum x and y values; `nx` is the number of intervals in the x coordinates (the number of steps in x direction is then `(xmax-xmin)/nx`); `ny` is the number of intervals in the y coordinates; `width` is the width of each column in the table (a positive integer); `decimals` is the number of decimals used when writing out the numbers (`None` means no decimal specification), and `filename` is the name of the output file. For example, `width=10` and `decimals=1` gives the output format `%10.1g`, while `width=5` and `decimals=None` implies `%5g`.

[13] http://tinyurl.com/pwyasaa/plot

Here is a test function which you should use to verify the implementation:

```
def test_write_table_to_file():
    filename = 'tmp.dat'
    write_table_to_file(f=lambda x, y: x + 2*y,
                        xmin=0, xmax=2, nx=4,
                        ymin=-1, ymax=2, ny=3,
                        width=5, decimals=None,
                        filename=filename)
    # Load text in file and compare with expected results
    with open(filename, 'r') as infile:
        computed = infile.read()
    expected = """\
    2    4  4.5    5  5.5    6
    1    2  2.5    3  3.5    4
    0    0  0.5    1  1.5    2
   -1   -2 -1.5   -1 -0.5    0

         0  0.5    1  1.5    2"""
    assert computed == expected
```

Filename: `write_table_to_file`.

Exercise 5.18: Fit a polynomial to data points

The purpose of this exercise is to find a simple mathematical formula for how the density of water or air depends on the temperature. The idea is to load density and temperature data from file as explained in Exercise 5.16 and then apply some NumPy utilities that can find a polynomial that approximates the density as a function of the temperature.

NumPy has a function `polyfit(x, y, deg)` for finding a best fit of a polynomial of degree `deg` to a set of data points given by the array arguments `x` and `y`. The `polyfit` function returns a list of the coefficients in the fitted polynomial, where the first element is the coefficient for the term with the highest degree, and the last element corresponds to the constant term. For example, given points in `x` and `y`, `polyfit(x, y, 1)` returns the coefficients `a, b` in a polynomial `a*x + b` that fits the data in the best way. (More precisely, a line $y = ax + b$ is a best fit to the data points (x_i, y_i), $i = 0, \ldots, n-1$ if a and b are chosen to make the sum of squared errors $R = \sum_{j=0}^{n-1}(y_j - (ax_j + b))^2$ as small as possible. This approach is known as *least squares approximation* to data and proves to be extremely useful throughout science and technology.)

NumPy also has a utility `poly1d`, which can take the tuple or list of coefficients calculated by, e.g., `polyfit` and return the polynomial as a Python function that can be evaluated. The following code snippet demonstrates the use of `polyfit` and `poly1d`:

```
coeff = polyfit(x, y, deg)
p = poly1d(coeff)
print p             # prints the polynomial expression
y_fitted = p(x)     # computes the polynomial at the x points
# Use red circles for data points and a blue line for the polyn.
plot(x, y, 'ro', x, y_fitted, 'b-',
     legend=('data', 'fitted polynomial of degree %d' % deg))
```

a) Write a function `fit(x, y, deg)` that creates a plot of data in `x` and `y` arrays along with polynomial approximations of degrees collected in the list `deg` as explained above.
b) We want to call `fit` to make a plot of the density of water versus temperature and another plot of the density of air versus temperature. In both calls, use `deg=[1,2]` such that we can compare linear and quadratic approximations to the data.
c) From a visual inspection of the plots, can you suggest simple mathematical formulas that relate the density of air to temperature and the density of water to temperature?

Filename: `fit_density_data`.

Exercise 5.19: Fit a polynomial to experimental data
Suppose we have measured the oscillation period T of a simple pendulum with a mass m at the end of a massless rod of length L. We have varied L and recorded the corresponding T value. The measurements are found in a file `src/plot/pendulum.dat`[14]. The first column in the file contains L values and the second column has the corresponding T values.

a) Plot L versus T using circles for the data points.
b) We shall assume that L as a function of T is a polynomial. Use the NumPy utilities `polyfit` and `poly1d`, as explained in Exercise 5.18, to fit polynomials of degree 1, 2, and 3 to the L and T data. Visualize the polynomial curves together with the experimental data. Which polynomial fits the measured data best?

Filename: `fit_pendulum_data`.

Exercise 5.20: Read acceleration data and find velocities
A file `src/plot/acc.dat`[15] contains measurements $a_0, a_1, \ldots, a_{n-1}$ of the acceleration of an object moving along a straight line. The measurement a_k is taken at time point $t_k = k\Delta t$, where Δt is the time spacing between the measurements. The purpose of the exercise is to load the acceleration data into a program and compute the velocity $v(t)$ of the object at some time t.

In general, the acceleration $a(t)$ is related to the velocity $v(t)$ through $v'(t) = a(t)$. This means that

$$v(t) = v(0) + \int_0^t a(\tau)d\tau\,. \tag{5.22}$$

If $a(t)$ is only known at some discrete, equally spaced points in time, $a_0, \ldots, a_{n-1}$ (which is the case in this exercise), we must compute the integral in (5.22) numerically, for example by the Trapezoidal rule:

$$v(t_k) \approx \Delta t\left(\frac{1}{2}a_0 + \frac{1}{2}a_k + \sum_{i=1}^{k-1} a_i\right), \quad 1 \leq k \leq n-1\,. \tag{5.23}$$

We assume $v(0) = 0$ so that also $v_0 = 0$.

[14] http://tinyurl.com/pwyasaa/plot/pendulum.dat
[15] http://tinyurl.com/pwyasaa/plot/acc.dat

Read the values $a_0, \ldots, a_{n-1}$ from file into an array, plot the acceleration versus time, and use (5.23) to compute one $v(t_k)$ value, where Δt and $k \geq 1$ are specified on the command line.
Filename: `acc2vel_v1`.

Exercise 5.21: Read acceleration data and plot velocities
The task in this exercise is the same as in Exercise 5.20, except that we now want to compute $v(t_k)$ for all time points $t_k = k\Delta t$ and plot the velocity versus time. Now only Δt is given on the command line, and the $a_0, \ldots, a_{n-1}$ values must be read from file as in Exercise 5.20.

Hint Repeated use of (5.23) for all k values is very inefficient. A more efficient formula arises if we add the area of a new trapezoid to the previous integral (see also Sect. A.1.7):

$$v(t_k) = v(t_{k-1}) + \int_{t_{k-1}}^{t_k} a(\tau)d\tau \approx v(t_{k-1}) + \Delta t \frac{1}{2}(a_{k-1} + a_k), \tag{5.24}$$

for $k = 1, 2, \ldots, n-1$, while $v_0 = 0$. Use this formula to fill an array `v` with velocity values.
Filename: `acc2vel`.

Exercise 5.22: Plot a trip's path and velocity from GPS coordinates
A GPS device measures your position at every s seconds. Imagine that the positions corresponding to a specific trip are stored as (x, y) coordinates in a file `src/plot/pos.dat`[16] with an x and y number on each line, except for the first line, which contains the value of s.

a) Plot the two-dimensional curve of corresponding to the data in the file.

Hint Load s into a `float` variable and then the x and y numbers into two arrays. Draw a straight line between the points, i.e., plot the y coordinates versus the x coordinates.

b) Plot the velocity in x direction versus time in one plot and the velocity in y direction versus time in another plot.

Hint If $x(t)$ and $y(t)$ are the coordinates of the positions as a function of time, we have that the velocity in x direction is $v_x(t) = dx/dt$, and the velocity in y direction is $v_y = dy/dt$. Since x and y are only known for some discrete times, $t_k = ks$, $k = 0, \ldots, n-1$, we must use numerical differentiation. A simple (forward) formula is

$$v_x(t_k) \approx \frac{x(t_{k+1}) - x(t_k)}{s}, \quad v_y(t_k) \approx \frac{y(t_{k+1}) - y(t_k)}{s}, \quad k = 0, \ldots, n-2\,.$$

[16] http://tinyurl.com/pwyasaa/plot/pos.dat

Compute arrays `vx` and `vy` with velocities based on the formulas above for $v_x(t_k)$ and $v_y(t_k)$, $k = 0, \ldots, n-2$.
Filename: `position2velocity`.

Exercise 5.23: Vectorize the Midpoint rule for integration
The Midpoint rule for approximating an integral can be expressed as

$$\int_a^b f(x)dx \approx h \sum_{i=1}^{n} f(a - \frac{1}{2}h + ih), \tag{5.25}$$

where $h = (b-a)/n$.

a) Write a function `midpointint(f, a, b, n)` to compute Midpoint rule. Use a plain Python `for` loop to implement the sum.
b) Make a vectorized implementation of the Midpoint rule where you compute the sum by Python's built-in function `sum`.
c) Make another vectorized implementation of the Midpoint rule where you compute the sum by the `sum` function in the `numpy` package.
d) Organize the three implementations above in a module file `midpoint_vec.py`. Equip the module with one test function for verifying the three implementations. Use the integral $\int_2^4 2xdx = 12$ as test case since the Midpoint rule will integrate such a linear integrand exactly.
e) Start IPython, import the functions from `midpoint_vec.py`, define some Python implementation of a mathematical function $f(x)$ to integrate, and use the `%timeit` feature of IPython to measure the efficiency of the three alternative implementations.

Hint The `%timeit` feature is described in Sect. H.8.1.
Filename: `midpoint_vec`.

Remarks The lesson learned from the experiments in e) is that `numpy.sum` is much more efficient than Python's built-in function `sum`. Vectorized implementations must always make use of `numpy.sum` to compute sums.

Exercise 5.24: Vectorize a function for computing the area of a polygon
The area of a polygon is given by (3.17) in Exercise 3.19. Vectorize this formula such that there are no Python loops in the implementation. Make a test function that compares the scalar implementation in the referred exercise with the new vectorized implementation for some chosen polygons (the scalar version must then be available in a module so that the function can be imported).

Hint Observe that the formula $x_1y_2 + x_2y_3 + \cdots + x_{n-1}y_n = \sum_{i=0}^{n-1} x_i y_{i+1}$ is the dot product of two vectors, `x[:-1]` and `y[1:]`, which can be computed as `numpy.dot(x[:-1], y[1:])`.
Filename: `polygon_area_vec`.

Exercise 5.25: Implement Lagrange's interpolation formula

Imagine we have $n+1$ measurements of some quantity y that depends on x: $(x_0, y_0), (x_1, y_1), \ldots, (x_n, y_n)$. We may think of y as a function of x and ask what y is at some arbitrary point x not coinciding with any of the points $x_0, \ldots, x_n$. It is not clear how y varies between the measurement points, but we can make assumptions or models for this behavior. Such a problem is known as *interpolation*.

One way to solve the interpolation problem is to fit a continuous function that goes through all the $n+1$ points and then evaluate this function for any desired x. A candidate for such a function is the polynomial of degree n that goes through all the points. It turns out that this polynomial can be written

$$p_L(x) = \sum_{k=0}^{n} y_k L_k(x), \tag{5.26}$$

where

$$L_k(x) = \prod_{i=0, i\neq k}^{n} \frac{x - x_i}{x_k - x_i}. \tag{5.27}$$

The $\prod$ notation corresponds to $\sum$, but the terms are multiplied. For example,

$$\prod_{i=0, i\neq k}^{n} x_i = x_0 x_1 \cdots x_{k-1} x_{k+1} \cdots x_n .$$

The polynomial $p_L(x)$ is known as Lagrange's interpolation formula, and the points $(x_0, y_0), \ldots, (x_n, y_n)$ are called interpolation points.

a) Make functions `p_L(x, xp, yp)` and `L_k(x, k, xp, yp)` that evaluate $p_L(x)$ and $L_k(x)$ by (5.26) and (5.27), respectively, at the point `x`. The arrays `xp` and `yp` contain the x and y coordinates of the $n+1$ interpolation points, respectively. That is, `xp` holds $x_0, \ldots, x_n$, and `yp` holds $y_0, \ldots, y_n$.

b) To verify the program, we observe that $L_k(x_k) = 1$ and that $L_k(x_i) = 0$ for $i \neq k$, implying that $p_L(x_k) = y_k$. That is, the polynomial p_L goes through all the points $(x_0, y_0), \ldots, (x_n, y_n)$. Write a function `test_p_L(xp, yp)` that computes $|p_L(x_k) - y_k|$ at all the interpolation points (x_k, y_k) and checks that the value is approximately zero. Call `test_p_L` with `xp` and `yp` corresponding to 5 equally spaced points along the curve $y = \sin(x)$ for $x \in [0, \pi]$. Thereafter, evaluate $p_L(x)$ for an x in the middle of two interpolation points and compare the value of $p_L(x)$ with the exact one.

Filename: `Lagrange_poly1`.

Exercise 5.26: Plot Lagrange's interpolating polynomial

a) Write a function

```
def graph(f, n, xmin, xmax, resolution=1001):
```

for plotting $p_L(x)$ in Exercise 5.25, based on interpolation points taken from some mathematical function $f(x)$ represented by the argument `f`. The argument `n` denotes the number of interpolation points sampled from the $f(x)$ function, and `resolution` is the number of points between `xmin` and `xmax` used to plot $p_L(x)$. The x coordinates of the `n` interpolation points can be uniformly distributed between `xmin` and `xmax`. In the graph, the interpolation points $(x_0, y_0), \ldots, (x_n, y_n)$ should be marked by small circles. Test the `graph` function by choosing 5 points in $[0, \pi]$ and `f` as $\sin x$.

b) Make a module `Lagrange_poly2` containing the `p_L`, `L_k`, `test_p_L`, and `graph` functions. The call to `test_p_L` described in Exercise 5.25 and the call to `graph` described above should appear in the module's test block.

Hint Section 4.9 describes how to make a module. In particular, a test block is explained in Sect. 4.9.3, test functions like `test_p_L` are demonstrated in Sect. 4.9.4 and also in Sect. 3.4.2, and how to combine `test_p_L` and `graph` calls in the test block is exemplified in Sect. 4.9.5.
Filename: `Lagrange_poly2`.

Exercise 5.27: Investigate the behavior of Lagrange's interpolating polynomials
Unfortunately, the polynomial $p_L(x)$ defined and implemented in Exercise 5.25 can exhibit some undesired oscillatory behavior that we shall explore graphically in this exercise. Call the `graph` function from Exercise 5.26 with $f(x) = |x|$, $x \in [-2, 2]$, for $n = 2, 4, 6, 10$. All the graphs of $p_L(x)$ should appear in the same plot for comparison. In addition, make a new figure with results from calls to `graph` for $n = 13$ and $n = 20$. All the code necessary for solving this exercise should appear in some separate program file, which imports the `Lagrange_poly2` module made in Exercise 5.26.
Filename: `Lagrange_poly2b`.

Remarks The purpose of the $p_L(x)$ function is to compute (x, y) between some given (often measured) data points $(x_0, y_0), \ldots, (x_n, y_n)$. We see from the graphs that for a small number of interpolation points, $p_L(x)$ is quite close to the curve $y = |x|$ we used to generate the data points, but as n increases, $p_L(x)$ starts to oscillate, especially toward the end points (x_0, y_0) and (x_n, y_n). Much research has historically been focused on methods that do not result in such strange oscillations when fitting a polynomial to a set of points.

Exercise 5.28: Plot a wave packet
The function

$$f(x, t) = e^{-(x-3t)^2} \sin(3\pi(x - t)) \tag{5.28}$$

describes for a fixed value of t a wave localized in space. Make a program that visualizes this function as a function of x on the interval $[-4, 4]$ when $t = 0$.
Filename: `plot_wavepacket`.

Exercise 5.29: Judge a plot
Assume you have the following program for plotting a parabola:

```
import numpy as np
x = np.linspace(0, 2, 20)
y = x*(2 - x)
import matplotlib.pyplot as plt
plt.plot(x, y)
plt.show()
```

Then you switch to the function $\cos(18\pi x)$ by altering the computation of y to `y = cos(18*pi*x)`. Judge the resulting plot. Is it correct? Display the $\cos(18\pi x)$ function with 1000 points in the same plot.
Filename: `judge_plot`.

Exercise 5.30: Plot the viscosity of water
The viscosity of water, μ, varies with the temperature T (in Kelvin) according to

$$\mu(T) = A \cdot 10^{B/(T-C)}, \tag{5.29}$$

where $A = 2.414 \cdot 10^{-5}$ Pa s, $B = 247.8$ K, and $C = 140$ K. Plot $\mu(T)$ for T between 0 and 100 degrees Celsius. Label the x axis with 'temperature (C)' and the y axis with 'viscosity (Pa s)'. Note that T in the formula for μ must be in Kelvin.
Filename: `water_viscosity`.

Exercise 5.31: Explore a complicated function graphically
The wave speed c of water surface waves depends on the length λ of the waves. The following formula relates c to λ:

$$c(\lambda) = \sqrt{\frac{g\lambda}{2\pi}\left(1 + s\frac{4\pi^2}{\rho g\lambda^2}\right)\tanh\left(\frac{2\pi h}{\lambda}\right)}. \tag{5.30}$$

Here, g is the acceleration of gravity (9.81 m/s^2), s is the air-water surface tension ($7.9 \cdot 10^{-2}$ N/m), ρ is the density of water (can be taken as 1000 kg/m^3), and h is the water depth. Let us fix h at 50 m. First make a plot of $c(\lambda)$ (in m/s) for small λ (0.001 m to 0.1 m). Then make a plot $c(\lambda)$ for larger λ (1 m to 2 km.
Filename: `water_wave_velocity`.

Exercise 5.32: Plot Taylor polynomial approximations to sin *x*
The sine function can be approximated by a polynomial according to the following formula:

$$\sin x \approx S(x;n) = \sum_{j=0}^{n}(-1)^j \frac{x^{2j+1}}{(2j+1)!}. \tag{5.31}$$

The expression $(2j+1)!$ is the factorial (`math.factorial` can compute this quantity). The error in the approximation $S(x;n)$ decreases as n increases and in the limit we have that $\lim_{n\to\infty} S(x;n) = \sin x$. The purpose of this exercise is to visualize the quality of various approximations $S(x;n)$ as n increases.

a) Write a Python function `S(x, n)` that computes $S(x;n)$. Use a straightforward approach where you compute each term as it stands in the formula, i.e.,

$(-1)^j x^{2j+1}$ divided by the factorial $(2j+1)!$. (We remark that Exercise A.14 outlines a much more efficient computation of the terms in the series.)

b) Plot $\sin x$ on $[0, 4\pi]$ together with the approximations $S(x;1)$, $S(x;2)$, $S(x;3)$, $S(x;6)$, and $S(x;12)$.

Filename: `plot_Taylor_sin`.

Exercise 5.33: Animate a wave packet
Display an animation of the function $f(x,t)$ in Exercise 5.28 by plotting f as a function of x on $[-6,6]$ for a set of t values in $[-1,1]$. Also make an animated GIF file.

Hint A suitable resolution can be 1000 intervals (1001 points) along the x axis, 60 intervals (61 points) in time, and 6 frames per second in the animated GIF file. Use the recipe in Sect. 5.3.4 and remember to remove the family of old plot files in the beginning of the program.
Filename: `plot_wavepacket_movie`.

Exercise 5.34: Animate a smoothed Heaviside function
Visualize the smoothed Heaviside function $H_\epsilon(x)$, defined in 3.26), as an animation where ϵ starts at 2 and then goes to zero.
Filename: `smoothed_Heaviside_movie`.

Exercise 5.35: Animate two-scale temperature variations
We consider temperature oscillations in the ground as addressed in Sect. 5.13.2. Now we want to visualize daily and annual variations. Let A_1 be the amplitude of annual variations and A_2 the amplitude of the day/night variations. Let also $P_1 = 365$ days and $P_2 = 24$ h be the periods of the annual and the daily oscillations. The temperature at time t and depth z is then given by

$$T(z,t) = T_0 + A_1 e^{-a_1 z} \sin(\omega_1 t - a_1 z) + A_2 e^{-a_2 z} \sin(\omega_2 t - a_2 z), \tag{5.32}$$

where

$$\begin{aligned} \omega_1 &= 2\pi P_1, \\ \omega_2 &= 2\pi P_2, \\ a_1 &= \sqrt{\frac{\omega_1}{2k}}, \\ a_2 &= \sqrt{\frac{\omega_2}{2k}}. \end{aligned}$$

Choose $k = 10^{-6}\,\mathrm{m}^2/\mathrm{s}$, $A_1 = 15$ C, $A_2 = 7$ C, and the resolution Δt as $P_2/10$. Modify the `heatwave.py` program in order to animate this new temperature function.
Filename: `heatwave2`.

Remarks We assume in this problem that the temperature T equals the reference temperature T_0 at $t = 0$, resulting in a sine variation rather than the cosine variation in (5.18).

Exercise 5.36: Use non-uniformly distributed coordinates for visualization
Watching the animation in Exercise 5.35 reveals that there are rapid oscillations in a small layer close to $z = 0$. The variations away from $z = 0$ are much smaller in time and space. It would therefore be wise to use more z coordinates close to $z = 0$ than for larger z values. Given a set $x_0 < x_1 < \cdots < x_n$ of uniformly spaced coordinates in $[a, b]$, we can compute new coordinates $\bar{x}_i$, stretched toward $x = a$, by the formula

$$\bar{x}_i = a + (b - a)\left(\frac{x_i - a}{b - a}\right)^s,$$

for some $s > 1$. In the present example, we can use this formula to stretch the z coordinates to the left.

a) Experiment with $s \in [1.2, 3]$ and few points (say 15) and visualize the curve as a line with circles at the points so that you can easily see the distribution of points toward the left end. Identify a suitable value of s.
b) Run the animation with no circles and (say) 501 points with the found s value.

Filename: `heatwave2a`.

Exercise 5.37: Animate a sequence of approximations to π
Exercise 3.18 outlines an idea for approximating π as the length of a polygon inside the circle. Wrap the code from that exercise in a function `pi_approx(N)`, which returns the approximation to π using a polygon with $N + 1$ equally distributed points. The task of the present exercise is to visually display the polygons as a movie, where each frame shows the polygon with $N + 1$ points together with the circle and a title reflecting the corresponding error in the approximate value of π. The whole movie arises from letting N run through $4, 5, 6, \ldots, K$, where K is some (large) prescribed value. Let there be a pause of 0.3 s between each frame in the movie. By playing the movie you will see how the polygons move closer and closer to the circle and how the approximation to π improves.
Filename: `pi_polygon_movie`.

Exercise 5.38: Animate a planet's orbit
A planet's orbit around a star has the shape of an ellipse. The purpose of this exercise is to make an animation of the movement along the orbit. One should see a small disk, representing the planet, moving along an elliptic curve. An evolving solid line shows the development of the planet's orbit as the planet moves and the title displays the planet's instantaneous velocity magnitude. As a test, run the special case of a circle and verify that the magnitude of the velocity remains constant as the planet moves.

Hint 1 The points (x, y) along the ellipse are given by the expressions

$$x = a\cos(\omega t), \quad y = b\sin(\omega t),$$

where a is the semi-major axis of the ellipse, b is the semi-minor axis, ω is an angular velocity of the planet around the star, and t denotes time. One complete orbit corresponds to $t \in [0, 2\pi/\omega]$. Let us discretize time into time points $t_k = k\Delta t$, where $\Delta t = 2\pi/(\omega n)$. Each frame in the movie corresponds to (x, y) points along the curve with t values $t_0, t_1, \ldots, t_i, i$ representing the frame number ($i = 1, \ldots, n$).

Hint 2 The velocity vector is

$$(\frac{dx}{dt}, \frac{dy}{dt}) = (-\omega a \sin(\omega t), \omega b \cos(\omega t)),$$

and the magnitude of this vector becomes $\omega\sqrt{a^2 \sin^2(\omega t) + b^2 \cos^2(\omega t)}$.
Filename: `planet_orbit`.

Exercise 5.39: Animate the evolution of Taylor polynomials
A general series approximation (to a function) can be written as

$$S(x; M, N) = \sum_{k=M}^{N} f_k(x)\,.$$

For example, the Taylor polynomial of degree N for e^x equals $S(x; 0, N)$ with $f_k(x) = x^k/k!$. The purpose of the exercise is to make a movie of how $S(x; M, N)$ develops and improves as an approximation as we add terms in the sum. That is, the frames in the movie correspond to plots of $S(x; M, M)$, $S(x; M, M + 1)$, $S(x; M, M + 2)$, ..., $S(x; M, N)$.

a) Make a function

```
animate_series(fk, M, N, xmin, xmax, ymin, ymax, n, exact)
```

for creating such animations. The argument `fk` holds a Python function implementing the term $f_k(x)$ in the sum, `M` and `N` are the summation limits, the next arguments are the minimum and maximum x and y values in the plot, `n` is the number of x points in the curves to be plotted, and `exact` holds the function that $S(x)$ aims at approximating.

Hint Here is some more information on how to write the `animate_series` function. The function must accumulate the $f_k(x)$ terms in a variable s, and for each k value, s is plotted against x together with a curve reflecting the exact function. Each plot must be saved in a file, say with names `tmp_0000.png`, `tmp_0001.png`, and so on (these filenames can be generated by `tmp_%04d.png`, using an appropriate counter). Use the `movie` function to combine all the plot files into a movie in a desired movie format.

In the beginning of the `animate_series` function, it is necessary to remove all old plot files of the form `tmp_*.png`. This can be done by the `glob` module and the `os.remove` function as exemplified in Sect. 5.3.4.

b) Call the `animate_series` function for the Taylor series for $\sin x$, where $f_k(x) = (-1)^k x^{2k+1}/(2k+1)!$, and $x \in [0, 13\pi]$, $M = 0$, $N = 40$, $y \in [-2, 2]$.
c) Call the `animate_series` function for the Taylor series for e^{-x}, where $f_k(x) = (-x)^k/k!$, and $x \in [0, 15]$, $M = 0$, $N = 30$, $y \in [-0.5, 1.4]$.

Filename: `animate_Taylor_series`.

Exercise 5.40: Plot the velocity profile for pipeflow
A fluid that flows through a (very long) pipe has zero velocity on the pipe wall and a maximum velocity along the centerline of the pipe. The velocity v varies through the pipe cross section according to the following formula:

$$v(r) = \left(\frac{\beta}{2\mu_0}\right)^{1/n} \frac{n}{n+1}\left(R^{1+1/n} - r^{1+1/n}\right), \tag{5.33}$$

where R is the radius of the pipe, β is the pressure gradient (the force that drives the flow through the pipe), μ_0 is a viscosity coefficient (small for air, larger for water and even larger for toothpaste), n is a real number reflecting the viscous properties of the fluid ($n = 1$ for water and air, $n < 1$ for many modern plastic materials), and r is a radial coordinate that measures the distance from the centerline ($r = 0$ is the centerline, $r = R$ is the pipe wall).

a) Make a Python function that evaluates $v(r)$.
b) Plot $v(r)$ as a function of $r \in [0, R]$, with $R = 1$, $\beta = 0.02$, $\mu_0 = 0.02$, and $n = 0.1$.
c) Make an animation of how the $v(r)$ curves varies as n goes from 1 and down to 0.01. Because the maximum value of $v(r)$ decreases rapidly as n decreases, each curve can be normalized by its $v(0)$ value such that the maximum value is always unity.

Filename: `plot_velocity_pipeflow`.

Exercise 5.41: Plot sum-of-sines approximations to a function
Exercise 3.21 defines the approximation $S(t; n)$ to a function $f(t)$. Plot $S(t; 1)$, $S(t; 3)$, $S(t; 20)$, $S(t; 200)$, and the exact $f(t)$ function in the same plot. Use $T = 2\pi$.
Filename: `sinesum1_plot`.

Exercise 5.42: Animate the evolution of a sum-of-sine approximation to a function
First perform Exercise 5.41. A natural next step is to animate the evolution of $S(t; n)$ as n increases. Create such an animation and observe how the discontinuity in $f(t)$ is poorly approximated by $S(t; n)$, even when n grows large (plot $f(t)$ in each frame). This is a well-known deficiency, called Gibb's phenomenon, when approximating discontinuous functions by sine or cosine (Fourier) series.
Filename: `sinesum1_movie`.

Exercise 5.43: Plot functions from the command line
For quickly getting a plot of a function $f(x)$ for $x \in [x_{\min}, x_{\max}]$ it could be nice to a have a program that takes the minimum amount of information from the command line and produces a plot on the screen and saves the plot to a file `tmp.png`. The usage of the program goes as follows:

Terminal
```
plotf.py "f(x)" xmin xmax
```

Plotting $e^{-0.2x}\sin(2\pi x)$ for $x \in [0, 4\pi]$ is then specified as

Terminal
```
plotf.py "exp(-0.2*x)*sin(2*pi*x)" 0 4*pi
```

Write the `plotf.py` program with as short code as possible (we leave it to Exercise 5.44 to test for valid input).

Hint Make x coordinates from the second and third command-line arguments and then use `eval` (or `StringFunction` from `scitools.std`, see Sects. 4.3.3 and 5.5.1) on the first argument.
Filename: `plotf`.

Exercise 5.44: Improve command-line input
Equip the program from Exercise 5.43 with tests on valid input on the command line. Also allow an optional fourth command-line argument for the number of points along the function curve. Set this number to 501 if it is not given.
Filename: `plotf2`.

Exercise 5.45: Demonstrate energy concepts from physics
The vertical position $y(t)$ of a ball thrown upward is given by $y(t) = v_0 t - \frac{1}{2}gt^2$, where g is the acceleration of gravity and v_0 is the velocity at $t = 0$. Two important physical quantities in this context are the potential energy, obtained by doing work against gravity, and the kinetic energy, arising from motion. The potential energy is defined as $P = mgy$, where m is the mass of the ball. The kinetic energy is defined as $K = \frac{1}{2}mv^2$, where v is the velocity of the ball, related to y by $v(t) = y'(t)$.

Make a program that can plot $P(t)$ and $K(t)$ in the same plot, along with their sum $P + K$. Let $t \in [0, 2v_0/g]$. Read m and v_0 from the command line. Run the program with various choices of m and v_0 and observe that $P + K$ is always constant in this motion. (In fact, it turns out that $P + K$ is constant for a large class of motions, and this is a very important result in physics.)
Filename: `energy_physics`.

Exercise 5.46: Plot a w-like function
Define mathematically a function that looks like the "w" character. Plot the function. Also write a formal test function that verifies the implementation.
Filename: `plot_w`.

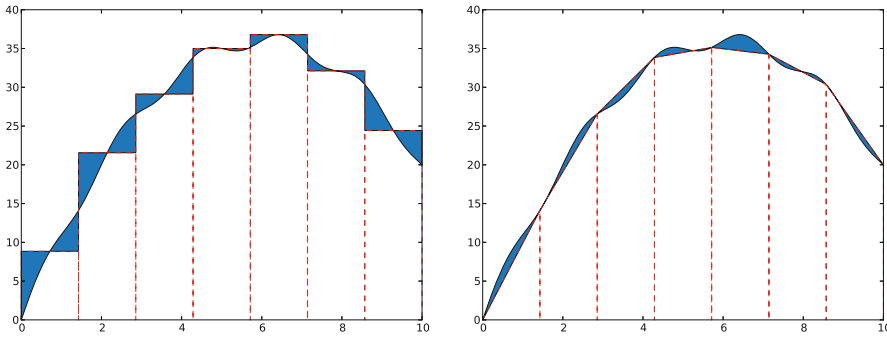


Fig. 5.22 Visualization of numerical integration rules, with the Midpoint rule to the left and the Trapezoidal rule to the right. The filled areas illustrate the deviations in the approximation of the area under the curve

Exercise 5.47: Plot a piecewise constant function
Consider the piecewise constant function defined in Exercise 3.32. Make a Python function `plot_piecewise(data, xmax)` that draws a graph of the function, where `data` is the nested list explained in mentioned exercise and `xmax` is the maximum x coordinate. Use ideas from Sect. 5.4.1.
Filename: `plot_piecewise_constant`.

Exercise 5.48: Vectorize a piecewise constant function
Consider the piecewise constant function defined in Exercise 3.32. Make a vectorized implementation `piecewise_constant_vec(x, data, xmax)` of such a function, where `x` is an array.

Hint You can use ideas from the `Nv1` function in Sect. 5.5.3. However, since the number of intervals is not known, it is necessary to store the various intervals and conditions in lists.
Filename: `piecewise_constant_vec`.

Remarks Plotting the array returned from `piecewise_constant_vec` faces the same problems as encountered in Sect. 5.4.1. It is better to make a custom plotting function that simply draws straight horizontal lines in each interval (Exercise 5.47).

Exercise 5.49: Visualize approximations in the Midpoint integration rule
Consider the midpoint rule for integration from Exercise 3.12. Use Matplotlib to make an illustration of the midpoint rule as shown to the left in Fig. 5.22.

The $f(x)$ function used in Fig. 5.22 is

$$f(x) = x(12 - x) + \sin(\pi x), \quad x \in [0, 10]\,.$$

Hint Look up the documentation of the Matplotlib function `fill_between` and use this function to create the filled areas between $f(x)$ and the approximating rectangles.

Note that the `fill_between` requires the two curves to have the same number of points. For accurate visualization of $f(x)$ you need quite many x coordinates,

and the rectangular approximation to $f(x)$ must be drawn using the same set of x coordinates.
Filename: `viz_midpoint`.

Exercise 5.50: Visualize approximations in the Trapezoidal integration rule
Redo Exercise 5.49 for the Trapezoidal rule from Exercise 3.11 to produce the graph shown to the right in Fig. 5.22.
Filename: `viz_trapezoidal`.

Exercise 5.51: Experience overflow in a function
We are give the mathematical function

$$v(x) = \frac{1 - e^{x/\mu}}{1 - e^{1/\mu}},$$

where μ is a parameter.

a) Make a Python function `v(x, mu=1E-6, exp=math.exp)` for calculating the formula for $v(x)$ using `exp` as a possibly user-given exponential function. Let the `v` function return the nominator and denominator in the formula as well as the fraction.
b) Call the `v` function for various `x` values between 0 and 1 in a `for` loop, let `mu` be `1E-3`, and have an inner `for` loop over two different `exp` functions: `math.exp` and `numpy.exp`. The output will demonstrate how the denominator is subject to overflow and how difficult it is to calculate this function on a computer.
c) Plot $v(x)$ for $\mu = 1, 0.01, 0.001$ on $[0, 1]$ using 10,000 points to see what the function looks like.
d) Convert `x` and `eps` to a higher precision representation of real numbers, with the aid of the NumPy type `float96`, before calling `v`:

```
import numpy
x = numpy.float96(x); mu = numpy.float96(e)
```

Repeat point b) with these type of variables and observe how much better results we get with `float96` compared with the standard `float` value, which is `float64` (the number reflects the number of bits in the machine's representation of a real number).
e) Call the `v` function with `x` and `mu` as `float32` variables and report how the function now behaves.

Filename: `boundary_layer_func1`.

Remarks When an object (ball, car, airplane) moves through the air, there is a very, very thin layer of air close to the object's surface where the air velocity varies dramatically, from the same value as the velocity of the object at the object's surface to zero a few centimeters away. This layer is called a *boundary layer*. The physics in the boundary layer is important for air resistance and cooling/heating of objects. The change in velocity in the boundary layer is quite abrupt and can be modeled by

the functiion $v(x)$, where $x = 1$ is the object's surface, and $x = 0$ is some distance away where one cannot notice any wind velocity v because of the passing object ($v = 0$). The wind velocity coincides with the velocity of the object at $x = 1$, here set to $v = 1$. The parameter μ is very small and related to the viscosity of air. With a small value of μ, it becomes difficult to calculate $v(x)$ on a computer. The exercise demonstrates the difficulties and provides a remedy.

Exercise 5.52: Apply a function to a rank 2 array
Let A be the two-dimensional array

$$\begin{bmatrix} 0 & 2 & -1 \\ -1 & -1 & 0 \\ 0 & 5 & 0 \end{bmatrix}$$

Apply the function f from Exercise 5.5 to each element in A. Then calculate the result of the array expression `A**3 + A*exp(A) + 1`, and demonstrate that the end result of the two methods are the same.
Filename: `apply_arrayfunc`.

Exercise 5.53: Explain why array computations fail
The following loop computes the array `y` from `x`:

```
>>> import numpy as np
>>> x = np.linspace(0, 1, 3)
>>> y = np.zeros(len(x))
>>> for i in range(len(x)):
...     y[i] = x[i] + 4
```

However, the alternative loop

```
>>> for xi, yi in zip(x, y):
...     yi = xi + 5
```

leaves `y` unchanged. Why? Explain in detail what happens in each pass of this loop and write down the contents of `xi`, `yi`, `x`, and `y` as the loop progresses.
Filename: `find_errors_arraycomp`.

Exercise 5.54: Verify linear algebra results
When we want to verify that a mathematical result is true, we often generate matrices or vectors with random elements and show that the result holds for these "arbitrary" mathematical objects. As an example, consider testing that $A + B = B + A$ for matrices A and B:

```
def test_addition():
    n = 4  # matrix size
    A = matrix(random.rand(n, n))
    B = matrix(random.rand(n, n))
```

```
    tol = 1E-14
    result1 = A + B
    result2 = B + A
    assert abs(result1 - result2).max() < tol
```

Use this technique to write test functions for the following mathematical results:

1. $(A + B)C = AC + BC$
2. $(AB)C = A(BC)$
3. $\text{rank}A = \text{rank}A^T$
4. $\det(AB) = \det A \det B$
5. The eigenvalues if A equals the eigenvalues of A^T when A is square.

Filename: `verify_linalg`.