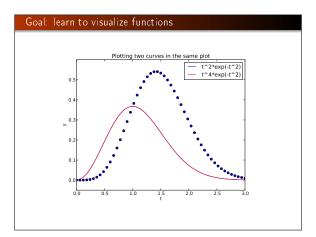
## Ch.5: Array computing and curve Plotting

Hans Petter Langtangen 1,2

Simula Research Laboratory <sup>1</sup>

University of Oslo, Dept. of Informatics <sup>2</sup>

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## We need to learn about a new object: array

- Curves y = f(x) are visualized by drawing straight lines between points along the curve
- Meed to store the coordinates of the points along the curve in lists or arrays x and y
- ullet Arrays pprox lists, but computationally much more efficient
- To compute the y coordinates (in an array) we need to learn about array computations or vectorization
- Array computations are useful for much more than plotting curves!

### The minimal need-to-know about vectors

- Vectors are known from high school mathematics, e.g., point (x, y) in the plane, point (x, y, z) in space
- In general, a vector v is an n-tuple of numbers:  $v = (v_0, \dots, v_{n-1})$
- Vectors can be represented by lists:  $v_i$  is stored as v[i], but we shall use arrays instead

Vectors and arrays are key concepts in this chapter. It takes separate math courses to understand what vectors and arrays really are, but in this course we only need a small subset of the complete story. A learning strategy may be to just start using vectors/arrays in programs and later, if necessary, go back to the more mathematical details in the first part of Ch. 5.

### The minimal need-to-know about arrays

Arrays are a generalization of vectors where we can have multiple indices:  $A_{i,j}$ ,  $A_{i,j,k}$ 

Example: table of numbers, one index for the row, one for the column  $% \left( 1\right) =\left( 1\right) \left( 1\right$ 

$$\begin{bmatrix} 0 & 12 & -1 & 5 \\ -1 & -1 & -1 & 0 \\ 11 & 5 & 5 & -2 \end{bmatrix} \qquad A = \begin{bmatrix} A_{0,0} & \cdots & A_{0} \\ \vdots & \ddots & \vdots \\ A_{m-1,0} & \cdots & A_{m-1} \end{bmatrix}$$

- The no of indices in an array is the rank or number of dimensions
- Vector = on e-dimensional array, or rank 1 array
- In Python code, we use Numerical Python arrays instead of nested lists to represent mathematical arrays (because this is computationally more efficient)

## Storing (x,y) points on a curve in lists Collect points on a function curve y = f(x) in lists: >>> def f(x): .... return x\*\*3 # sample function >>> a = 5>>> dx = 1.0/(a = 1) # sepacing in [0,1] >>> xlist = [i\*dx for i in range(n)] >>> plist = [f(x) for x in xlist] >>> pairs = [[x, y] for x, y in zip(xlist, ylist)] Turn lists into Numerical Python (NumPy) arrays: >>> import numpy as np >>> x2 = np array(xlist) >>> y2 = np array(ylist) # turn list xlist into array >>> y2 = np array(ylist)

## The pro drops lists and makes NumPy arrays directly: >>> n = 5 >>> x2 = np. linspace(0, 1, n) # n points in [0, 1] >>> y2 = np. zeros(n) >>> for i in xrange(n): ... y2[i] = f(x2[i]) ... Note: • xrange is like range but faster (esp. for large n - xrange does not explicitly build a list of integers, xrange just lets you loop over the values) • Entire arrays must be made by numpy (np) functions

```
Arrays are not as flexible as list, but computational much more efficient

• List elements can be any Python objects
• Array elements can only be of one object type
• Arrays are very efficient to store in memory and compute with if the element type is float, int, or complex
• Rule: use arrays for sequences of numbers
```

```
We can work with entire arrays at once - instead of one element at a time

Typical code for taking the sine of a list (or array) x by working with one element at a time:

for i in xrange(len(x)):
 y[i] = sin(x[i])

However, if x is array, y can be computed by
 y = np.sin(x)

# s: array, y: array

The loop is now inside np.sin and implemented in very efficient C code.
```

```
Vectorization gives:

• shorter, more readable code, closer to the mathematics
• much faster code

Use %timeit in IPython to measure the speed-up for y = sin xe<sup>-x</sup>:

In [1]: n = 100000

In [2]: import numpy as np

In [3]: x = np.linspace(0, 2*np.pi, n+1)  # n intervals in [0,2*pi]

In [4]: y = np.zeros(len(x))

In [5]: %timeit for i in xrange(len(x)): y[i] = np.sin(x[i])*np.exp
1 loops, best of 3: 247 ms per loop

In [6]: %timeit y = np.sin(x)*np.exp(-x)
100 loops, best of 3: 4.77 ms per loop

In [7]: 247/4.77

Out [7]: 51.781970649895186  # vectorization: 50x speed-up!
```

```
Array arithmetics is broken down to a series of unary/binary
array operations
     • Consider y = f(x), where f returns
      x**3 + sin(x)*exp(-3*x)
     • f(x) leads to the following set of vectorized
      sub-computations:
        for i in range(len(x)): r1[i] = x[i]**3 (but with
          loop in C)

    r2 = sin(x) (unary op, computed elementwise, but with loop

          in C)
        • r4 = exp(r3) (unary op.)
        5 r5 = r3*r4 (binary op.)
        0 r6 = r1 + r5 (binary op.)
        y = r6
     • Note: this is the same set of operations as you would do with
       a calculator when x is a number
```

## Important application: vectorized code for computing points along a curve

$$f(x) = x^2 e^{-\frac{1}{2}x} \sin(x - \frac{1}{3}\pi), \quad x \in [0, 4\pi]$$

from numpy import \* # Vectorized computation of 101 points along the curve x = linspace(0, 4\*pi, 101) y = 2.5 + x\*\*2\*exp(-0.5\*x)\*sin(x-pi/3)

### Vectorization

## Term in ology

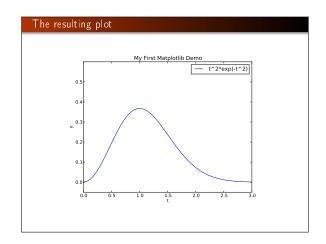
- Scalar: a number
- Vector or array: sequence of numbers (vector in mathematics)
- We speak about scalar computations (one number at a time) versus vectorized computations (operations on entire arrays, no Python loops)
- Functions that can operate on vectors (arrays) are called vectorized functions
- Vectorized functions are (usually) built of vectorized unary/binary operations
- Vectorization is the process of turning a non-vectorized algorithm with (Python) loops into a vectorized version without (Python) loops
- Mathematical functions in Python without if tests automatically work for both scalar and vector (array)

arguments (i.e. no vectorization is needed by the programmer

## Plotting the curve of a function: the very basics from scitools.std import \* # import numpy and plotting # Make points along the curve t = linspace(0, 3, 51) # 50 intervals in [0, 3] y = t\*\*2\*exp(-t\*\*2) # vectorized expression plot(t, y) # make plot on the screen savefig('fig.pdf') # make PNF image for reports savefig('fig.png') # make PNF image for web pages

## A plot should have labels on axis and a title

```
from scitools.std import * # import numpy and plotting
def f(t):
      return t**2*exp(-t**2)
t = linspace(0, 3, 51) # t coordinates
y = f(t) # corresponding
                                        # corresponding y values
plot(t, y)
 xlabel('t')
                                        # label on the x axis
| Ylabel('y') | Habel on the y axix | legend('t^2*exp(-t^2)') | # mark the curve | axis([0, 3, -0.05, 0.6]) # [tmin, tmax, ymin, ymax] | title('My First Easyviz Demo')
```



## SciTools vs. NumPy and Matplotlib

- SciTools is a Python package with lots of useful tools for mathematical computations, developed here in Oslo (Langtangen, Ring, Wilbers, Bredesen, ...)
- Easyviz is a subpackage of SciTools (scitools.easyviz) doing plotting with Matlab-like syntax
- Easyviz can use many plotting engine to produce a plot: Matplotlib, Gnuplot, Grace, Matlab, VTK, Open Dx, ... but the syntax remains the same
- Matplotlib is the standard plotting package in the Python community - Easyviz can use the same syntax as Matplotlib

```
from scitools.std import *
# is ca equivalent to
from numpy import *
from matplotlib.pyplot import *
```

## 

```
Plotting several curves in one plot

Plot t<sup>2</sup>e<sup>-t<sup>2</sup></sup> and t<sup>4</sup>e<sup>-t<sup>2</sup></sup> in the same plot:

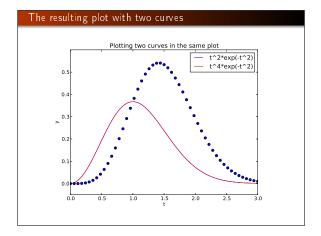
from scitcols.std import * # curve plotting + array computing

def fi(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)
hold('on') # continue plotting in the same plot
plot(t, y2)
xlabel('yt')
ylabel('yt')
legend('t-2*exp(-t-2)', 't-4*exp(-t-2)')
title('Plotting two curves in the same plot')
savefig('tmp2.png')
```



```
When plotting multiple curves in the same plot, the different lines (normally) look different. We can control the line type and color, if desired:

plot(t, y1, 'r-')  # red (r) line (-)
hold('on')
plot(t, y2, 'bo')  # blue (b) circles (o)

# or
plot(t, y1, 'r-', t, y2, 'bo')

Documentation of colors and line styles: see the book, Ch. 5, or
Unix> pydoc scitools.easyviz

for
```

```
Quick plotting with minimal typing

A lazy pro would do this:

t = linepace(0, 3, 51)
plot(t, t**2*exp(-t**2), t, t**4*exp(-t**2))
```

## 

# Complete program: from scitools.std import \* # or alternatively from numpy import \* from matplotlib.pyplot import \* formula = sys.argy[1] xmin = eval(sys.argy[2]) xmax = eval(sys.argy[3]) x = linspace(xmin, xmax, 101) y = eval(formula) plot(x, y, title=formula)

```
Let's make a movie/animation

The Gaussian bell function:

f(x; m, s) = \frac{1}{\sqrt{2\pi}} \frac{1}{s} \exp\left[-\frac{1}{2} \left(\frac{x-m}{s}\right)^2\right]
• m is the location of the peak
• s is a measure of the width of the function
• Make a movie (animation) of how f(x; m, s) changes shape as s goes from 2 to 0.2
```

```
Goal: make a movie showing how f(x) varies in shape as s decreases
Idea: put many plots (for different s values) together (exactly as a cartoon movie)
How to program: loop over s values, call plot for each s and make hardcopy, combine all hardcopies to a movie
Very important: fix the y axis! Otherwise, the y axis always adapts to the peak of the function and the visual impression gets completely wrong
```

```
The complete code for making the animation

from scitools.std import *
import time

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

m = 0;    s_start = 2;    s_stop = 0.2
    s_values = linspace(s_start, s_stop, 30)

x = linspace(m -3*s_start, m + 3*s_start, 1000)
    # f :s max for a*m (smaller s gives larger max value)
    max f = f(m, m, s_stop)

# Show the movie on the screen
# and make hardcopies of frames simultaneously
import time
frame_counter = 0

for s in s_values:
    y = f(x, m, s)
    plot(x, y, axis=[x[0], x[-i], -0.i, max_f],
        xlabel='x', ylabel='f', legend='s='WA 2f' % s,
        savetig='tmp_\( \lambda \) ang' % frame_counter)

frame_counter *= 1
    #time.sleep(0.2) # pause to control movie speed
```

```
We now have a lot of files:

tmp_0000.png tmp_0001.png tmp_0002.png ...

We use some program to combine these files to a video file:

convert for animted GIF format (if we have just a few plot files)

avconv for MP4, WebM, Ogg, and Flash formats
```

## Make and play animated GIF file Tool: convert from the ImageMagick software suite. Unix command: Terminal> convert -delay 50 tmp\_\*.png movie.gif Delay: 50/100 s, i.e., 0.5 s between each frame. Play animated GIF file with animate from ImageMagick: Terminal> animate movie.gif or insert this HTML code in some file tmp.html loaded into a browser: <image src="movie.gif">

```
Making MP4, Ogg, WebM, or Flash videos

Tool: avconv or ffmpeg

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

where

• -r 5 specifies 5 frames per second
• -i tmp_%04d.png specifies filenames
(tmp_0000.png, tmp_0001.png, ...)

Different formats apply different codecs (-vcodec) and video filenamet extensions:
Format Codec and filename
Flash -vcodec flv movie.flv
MP4 -vcodec libx264 movie.mp4
Webm -vcodec libvyx movie.webm
Ogg -vcodec libtheora movie.ogg
```

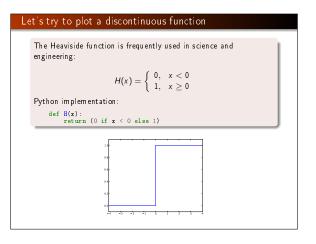
```
How to play movie files in general

Terminal> vlc movie.flv
Terminal> vlc movie.ogg
Terminal> vlc movie.webm
Terminal> vlc movie.mp4

Other players (on Linux) are mplayer, totem, ...
```

```
Terminal> scitools movie output_file=mymovie.html fps=4 tmp_*.png
makes a player of tmp_*.png files in a file mymovie.html (load
into a web browser), 4 frames per second
```

```
    It is possible to plot curves in pure text (!)
    ● Plots are stored in image files of type PDF, PNG, JPEG, or GIF
    ● Sometimes you want a plot to be included in your program, e.g., to prove that the curve looks right in a compulsory exercise where only the program (and not a nicely typeset report) is submitted
    ● scitools.aplotter can then be used for drawing primitive curves in pure text (ASCII) format
    >>> from scitools.aplotter import plot
    >>> x = linepace(-2, 2, 6i)
    >>> y = exp(-0.5xx*2)*cos(pi*x)
    >>> plot(x, y)
    Try these statements out!
```



```
Standard approach:

x = linspace(-10, 10, 5)  # few points (simple curve)
y = H(x)
plot(x, y)

First problem: ValueError error in H(x) from if x < 0
Let us debug in an interactive shell:

>>> x = linspace(-10,10,5)
>>> x
array([-10, -5., 0., 5., 10.])
>>> b = x < 0
>>> b
array([ True, True, False, False, False], dtype=bool)
>>> bool(b) # evaluate b in a boolean contest

ValueError: The truth value of an array with more than one element is ambiguous. Use a any() or a all()
```

```
Remedy 1: use a loop over x values

def H_loop(x):
    r = zeros(len(x))  # or r = z.copy()
    for i in xrange(len(x)):
        r[i] = H(x[i])
    return r

n = 5
x = linspace(-5, 5, n+1)
y = H_loop(x)

Downside: much to write, slow code if n is large
```

```
Remedy 2: use vectorize

from numpy import vectorize

# Automatic vectorization of function #
Hv = vectoriza(H)

# Hv(x) works with array x

Downside: The resulting function is as slow as Remedy 1
```

```
Remedy 3: code the if test differently
    def Hv(x):
        return where(x < 0, 0.0, 1.0)

More generally:
    def f(x):
        if condition:
            x = <expression1>
        else:
            x = <expression2>
        return x

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

```
With a vectorized Hv(x) function we can plot in the standard way

x = linspace(-10, 10, 5) # linspace(-10, 10, 50)

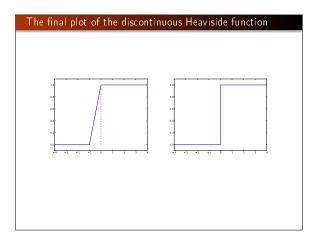
y = Hv(x)
plot(x, y, axis=[x[0], x[-1], -0.1, 1.1])
```

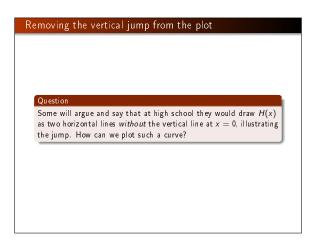
```
How to make the function look discontinuous in the plot?

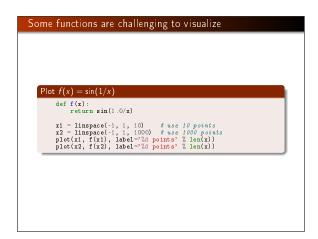
• Newbie: use a lot of x points; the curve gets steeper
• Pro: plot just two horizontal line segments one from x=-10 to x=0, y=0; and one from x=0 to x=10, y=1

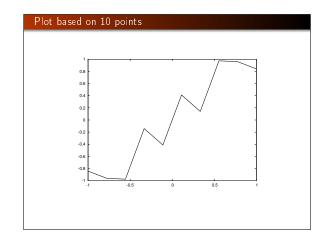
plot([-10, 0, 0, 10], [0, 0, 1, 1], aris=[x[0], x[-1], -0.1, 1.1])

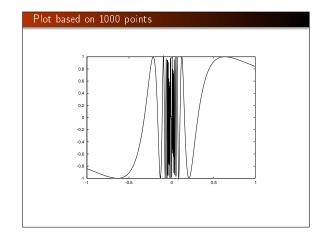
Draws straight lines between (-10,0), (0,0), (0,1), (10,1)
```











```
The two following statements are mathematically equivalent:

a = a + b  # a and b are arrays
a + b

However,

a = a + b is computed as (extra array needed)

or 1 = a + b
a = r1

a + b is computed as a[i] += b[i] for i in all indices (i.e., not extra array)

a += b is an in-place addition, because we change each element in a, rather than letting the name a refer to a new array, the result of a+b
```

```
Consider

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

Here are the actual computations in the computer:

r1 = x**4; r2 = 3*r1; r3 = 2*x; r4 = r1 + r3

r5 = r4 + 4; r6 - x + 1; r7 = r5/r6; a = r7

With in-place arithmetics we can save four extra arrays, though at the cost of much less readable code:

a = x.copy()

a **= 3

a += 2*x

a += 4

a /= x + 1
```

```
In-place arithmetics only saves memory, no significant speed-up

Let's use l'Python to measure the computational time:

In [1]: def expression(x):
...: return (3*x**4 + 2*x + 4)/(x + 1)
...: a = x.copy()
...: a = x.copy()
...: a **= 3
...: a **= 3
...: a **= 3
...: a **= 2*x
...: a **= 4
...: a **= 1
...: return a
...:

In [3]: import numpy as np
In [4]: x = np.linspace(0, 1, 10000000)
In [5]: %timeit expression(x)
1 loops, best of 3: 771 ms per loop
In [6]: %timeit expression_inplace(x)
1 loops, best of 3: 728 ms per loop
```

```
Useful array operations

Make a new array with same size as another array:

from numpy import *

# z is numpy array
a = x.copy()

# or
a = zeros(x.shape, x.dtype)

# or
a = zeros_like(x)  # zeros and same size as z

Make sure a list or array is an array:
a = asarray(a)
b = asarray(somearray, dtype=float)  # specify data type

Test if an object is an array:

>>> type(a)

<type 'numpy.ndarray'>
>>> isinstance(a, ndarray)

True
```

```
Recall slicing: a [f:t:i], where the slice f:t:i implies a set of indices (from, to, increment).

Any integer list or array can be used to indicate a set of indices:

>>> a = 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 [array([ 1, 10., 3., 4., 5., 6., 10., 10.])
>>> a [array([ 1., 10., 3., 4., 5., 6., 10., 10.])
>>> array([ 1., 10., -2., 4., 5., -2., 10., 10.])
```

Generalized array indexing

## Generalized array indexing with boolean expressions

## Two-dimensional arrays; math intro

When we have a table of numbers,

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

(called matrix by mathematicians) it is natural to use a two-dimensional array  $A_{i,j}$  with one index for the rows and one for the columns:

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

## Two-dimensional arrays; Python code

```
Making and filling a two-dimensional NumPy array goes like this:
```

```
A = zeros((3,4)) # 3x4 table of numbers
A[0,0] = -1
A[1,0] = 1
A[2,0] = 10
A[0,1] = -5
...
A[2,3] = -100
# can also write (as for nested lists)
A[2][3] = -100
```

## From nested list to two-dimensional array

```
Let us make a table of numbers in a nested list:

>>> 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]]

Turn into NumPy array:
>>> table2 = array(table)
>>> print table2
[[-30, -22.]
[-20, -4.]
[-10, 14.]]
```

## How to loop over two-dimensional arrays

## How to take slices of two-dimensional arrays

```
Time for a question
   Problem
   Given
        >>> 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.]])
   What will t [1:-1:2, 2:] be?
   Solution:
   Slice 1:-1:2 for first index results in
          [ 7., 8., 9., 10., 11., 12.]
[ 19., 20., 21., 22., 23., 24.]
   Slice 2: for the second index then gives
          [ 9., 10., 11., 12.]
[ 21., 22., 23., 24.]
```

```
Summary of vectors and arrays
     • Vector/array computing: apply a mathematical expression to
       every element in the vector/array (no loops in Python)
     • Ex: \sin(x**4)*\exp(-x**2), x can be array or scalar
       for array the i'th element becomes
       sin(x[i]**4)*exp(-x[i]**2)
     • Vectorization: make scalar mathematical computation valid for
       vectors/arrays
     • Pure mathematical expressions require no extra vectorization
     • Mathematical formulas involving if tests require manual work
       for vectorization:
       scalar_result = expression1 if condition else expression2
       vector_result = where(condition, expression1, expression2)
```

```
Summary of plotting y = f(x) curves
     Curve plotting (unified syntax for Matplotlib and SciTools):
            from matplotlib.pyplot import *
            #from scitools.std import *
            plot(x, y)
                                         # simplest command
           plot(t1, y1, 'r', f curve l, red line
t2, y2, 'b', f curve 2, blue line
t3, y3, 'o') f curve 3, circles at data points
axis([t1[0], t1[-1], -1.1, 1.1])
legend(['model 1', 'model 2', 'measurements'])
xlabel('time'); ylabel('force')
savefig('myframe_%04d.png' % plot_counter)
     Note: straight lines are drawn between each data point
```

```
Alternative plotting of y = f(x) curves
       Single SciTools plot command with keyword arguments:
               from scitools.std import *
              plot(t1, y1, 'r',  # curve 1, red line
    t2, y2, 'b',  # curve 2, blue line
    t3, y3, 'o',  # curve 3, circles at data points
    aris=[t1[0], t1[-1], -1.1, 1.1],
    legend=('model 1', 'model 2', 'measurements'),
    xlabel='time', ylabel='force',
    savefig='myframe_%04d.png' % plot_counter)
```

```
Summary of making animations

    Make a hardcopy of each plot frame (PNG or PDF format)

     • Use avconv or ffmpeg to make movie
      Terminal> avconv -r 5 -i tmp_%04d.png -vcodec flv movie.flv
```

```
Array functionality
           Construction
                                                      Meaning
                                 copy list data 1d to a numpy array
    array(ld)
    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
                                 make a two-dimensional float array with shape (m, 'n
    zeros((m,n))
    zeros_like(x)
                                 make array of same shape and element type as x
                                 uniform sequence of m numbers in [a, b]
    linspace(a,b,m)
    a.shape
                                 tuple containing a's shape
                                 total no of elements in a
    a.size
                                 length of a one-dim. array a (same as a. shape [0])
    len(a)
    a.dtype
                                 the type of elements in a
    a.reshape(3,2)
                                 return a reshaped as 3 \times 2 array
    a[i]
                                 vector indexing
                                two-dim. array indexing
    a[i,j]
    a[1:k]
                                 slice: reference data with indices 1,..., k-1'
    a[1:8:3]
                                 slice: reference data with indices 1, 4,...,'7'
                                copy an array
    b = a.copy()
    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
```

## Summarizing example: animating a function (part 1) • Goal: visualize the temperature in the ground as a function of depth (z) and time (t), displayed as a movie in time: $T(z,t) = T_0 + Ae^{-az}\cos(\omega t - az), \quad a = \sqrt{\frac{\omega}{2k}}$ • First we make a general animation function for an f(x,t): $\det x = \int_0^\infty \int_0$