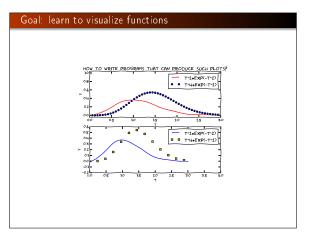
## Ch.5: Array computing and curve plotting

Hans Petter Langtangen 1,2

Simula Research Laboratory <sup>1</sup>

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

Aug 21, 2016



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

- Curves y = f(x) are visualized by drawing straight lines between points along the curve
- $\bullet$  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  $% \left( 1\right) =\left( 1\right) \left( 1\right$ 

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

- The no of indices in an array is the rank or number of dimensions
- Vector = one-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:

### Turn lists into Numerical Python (NumPy) arrays:

```
>>> import numpy as np  # module for arrays
>>> x = np.array(xlist)  # turn list wlist into array
>>> y = np.array(ylist)
```

# The pro drops lists and makes NumPy arrays directly: >>> n = 5 >>> x = np.linspace(0, 1, n) # n points in [0, 1] >>> for i in xrange(n): ... y[i] = f(x[ii]) ... 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

Compute the sine of an array:
 from math import sin
 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)

# x: array, y: array

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

```
Operating on entire arrays at once is called vectorization

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^-x:

In [1]: n = 100000

In [2]: import numpy as np

In [3]: x = np.linspace(0, 2*np.pi, n+i)

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

In [5]: "timeit for i in xrange(len(x)): \
y[i] = np.sin(x[i])*np.exp(-x[i])
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:
         0 r1 = x**3
           for i in range(len(x)): r1[i] = x[i]**3
           (but with loop in C)
         \bigcirc r2 = sin(x) (computed elementwise in C)
         0 \text{ r3} = -3*x
         0 \text{ r4} = \exp(\text{r3})
         0 \text{ r6} = \text{r1} + \text{r5}
         y = r6
     • Note: this is the same set of operations as you would do with
       a calculator when x is a number
```

## Very important application: vectorized code for computing points along a curve

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

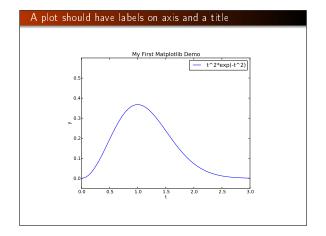
Vectorized computation of n+1 points along the curve from numpy import \*

```
n = 100
x = linspace(0, 4*pi, n+1)
y = 2.5 + x**2*exp(-0.5*x)*sin(x-pi/3)
```

### New term: vectorization

- 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)
- Vectorized functions can operate on arrays (vectors)
- 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 Plot the curve of $y(t) = t^2e^{-t^2}$ : 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 PDF image for reports savefig('fig.png') # make PDF image for web pages



```
The code that makes the last plot

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 y values

plot(t, y)

xlabel('t')  # label on the x axis
ylabel('t')  # label on the y axis
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, OpenDx, ... 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 basically equivalent to
from numpy import *
from matplotlib.pyplot import *
```

Note: SciTools (by default) adds markers to the lines, Matplotlib

```
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 scitools.std import * f curve plotting + array computing

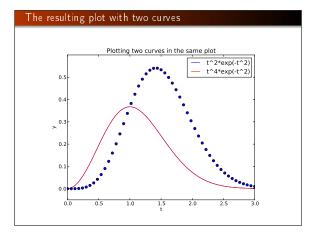
def f1(t):
    return t**2*exp(-t**2)

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

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

plot(t, y1)
hold('on') f continue plotting in the same plot
plot(t, y2)

xlabel('t')
ylabel('y')
legend('t-2*exp(-t-2)', 't-4*exp(-t-2)')
title('Plotting two curves in the same plot')
savefig('tmp2.png')
```

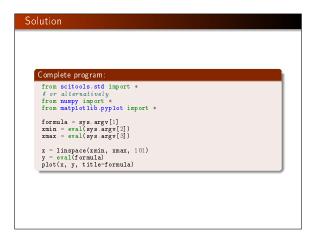


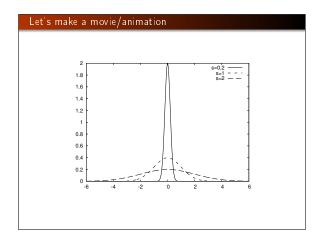
```
Quick plotting with minimal typing

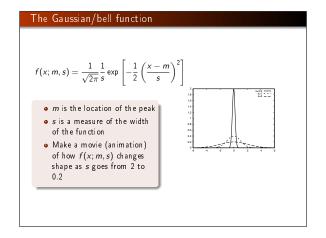
A lazy pro would do this:

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

## Plot function given on the command line Task: plot function given on the command line Terminal> python plotf.py expression xmin xmax Terminal> python plotf.py "exp(-0.2\*x)\*sin(2\*pi\*x)" 0.4\*pi Should plot $e^{-0.2x}\sin(2\pi x)$ , $x \in [0,4\pi]$ . plotf.py should work for "any" mathematical expression.







```
Movies are made from a (large) set of individual plots
```

- 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

## 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 just a few plot files) ffmpeg (or 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: <img src="movie.gif">

# Making MP4, Ogg, WebM, or Flash videos Tool: ffmpeg or avconv Terminal> ffmpeg -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 filename extensions: Forma Codec and filename Flash -vcodec flv movie.flv MP4 -vcodec libx264 movie.mp4 Webm -vcodec libyx movie.rebm Ogg -vcodec libtheora movie.ogg



```
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)
```

```
■ Plots are stored in image files of type PDF and PNG
■ 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
>>> from numpy import linspace, exp, cos, pi
>>> x = linspace(-2, 2, 81)
>>> y = exp(-0.5x**e2)*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 = x.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

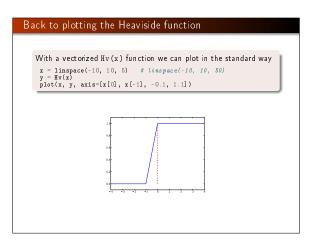
# Automatic vectorization of function H
Hv = vectorize(H)
# Hv(w) works with array w

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

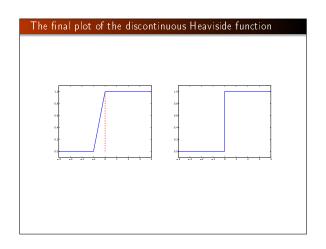
```
Remedy 3: code the if test differently
  def Hv(x):
    return where(x < 0, 0.0, 1.0)

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

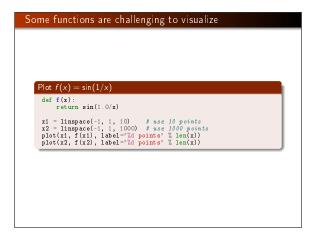
def f_vectorized(x):
  def f_vectorized(x):
    xi = <expression1>
    x2 = <expression2>
    return x
```

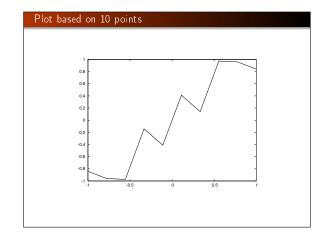


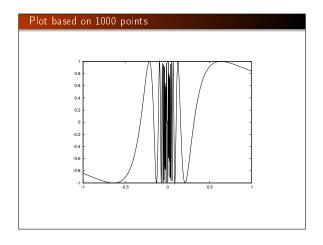
# Newbie: use a lot of x points; the curve gets steeper Pro: plot just two horizontal line segments one from x = -10 to x = 0, y = 0; and one from x = 0 to x = 10, y = 1 plot([-10, 0, 0, 10], [0, 0, 1, 1], axis=[x[0], x[-1], -0.1, 1.1]) Draws straight lines between (-10,0), (0,0), (0,1), (10,1)



## Removing the vertical jump from the plot $\frac{\text{Question}}{\text{Some will argue and say that at high school they would draw } H(x) \\ \text{as two horizontal lines } \textit{without the vertical line at } x=0, \text{ illustrating the jump. How can we plot such a curve?}$







```
Assignment of an array does not copy the elements!

a = x
a[-1] = 1000

ls x[-1] also changed to 1000?

Yes, because a refers to the same array as x.

Avoid changing x by letting a be a copy of x:
a = x.copy()

The same yields slices:

a = x[x:]  # a refers to a part of the x array
a[-1] = 1000  # changes x[-1]!

a = x[x:].copy()
a[-1] = 1000  # does not change x[-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) • r1 = 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 **= 4
a *= 3
a += 2*x
a += 4
a /= x + 1
```

```
Useful array operations

Make a new array with same size as another array:

from numpy import *

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

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

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

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
```

```
def f(x):
    return 2

Vectorized version must return array of 2's:
    def fv(x):
        return zeros(x.shape, x.dtype) + 2

New version valid both for scalar and array x:
    def f(x):
        if isinstance(x, (float, int)):
            return zeros(x.shape, x.dtype) + 2
    elif isinstance(x, ndarray):
            return zeros(x.shape, x.dtype) + 2
    else:
        raise TypeError(
            'x must be int/float/ndarray, not %s' % type(x))
```

## Generalized array indexing

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:

```
Any integer ist of ariay can be used to indicate a set of indic

>>> 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[range(2,8,3)] = -2 # same as a[2:8:3] = -2

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

## 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:

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

## 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

## 

```
    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)
```

```
    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 array(ld) copy list data 1d to a numpy array make array of data d (no data copy if already array) asarray(d) 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 linspace(a,b,m) uniform sequence of m numbers in [a, b] a.shape tuple containing a's shape total no of elements in a a.size len(a) length of a one-dim. array a (same as a. shape [0]) the type of elements in a a.dtype a.reshape(3,2) return a reshaped as $3 \times 2$ array a[i] vector indexing a[i,j] two-dim. array indexing a[1:k] slice: reference data with indices 1,..., k-1' slice: reference data with indices 1, 4,...,'7' a[1:8:3] 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

## 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):

Then we call this function with our special T(z,t) function