Slides from INF3331 lectures - numerical Python

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Numerical Python

Contents

More info

- Ch. 4 in the course book
- www.scipy.org
- scipy.github.com
- The NumPy manual
- The SciPy tutorial

Numerical Python (NumPy)

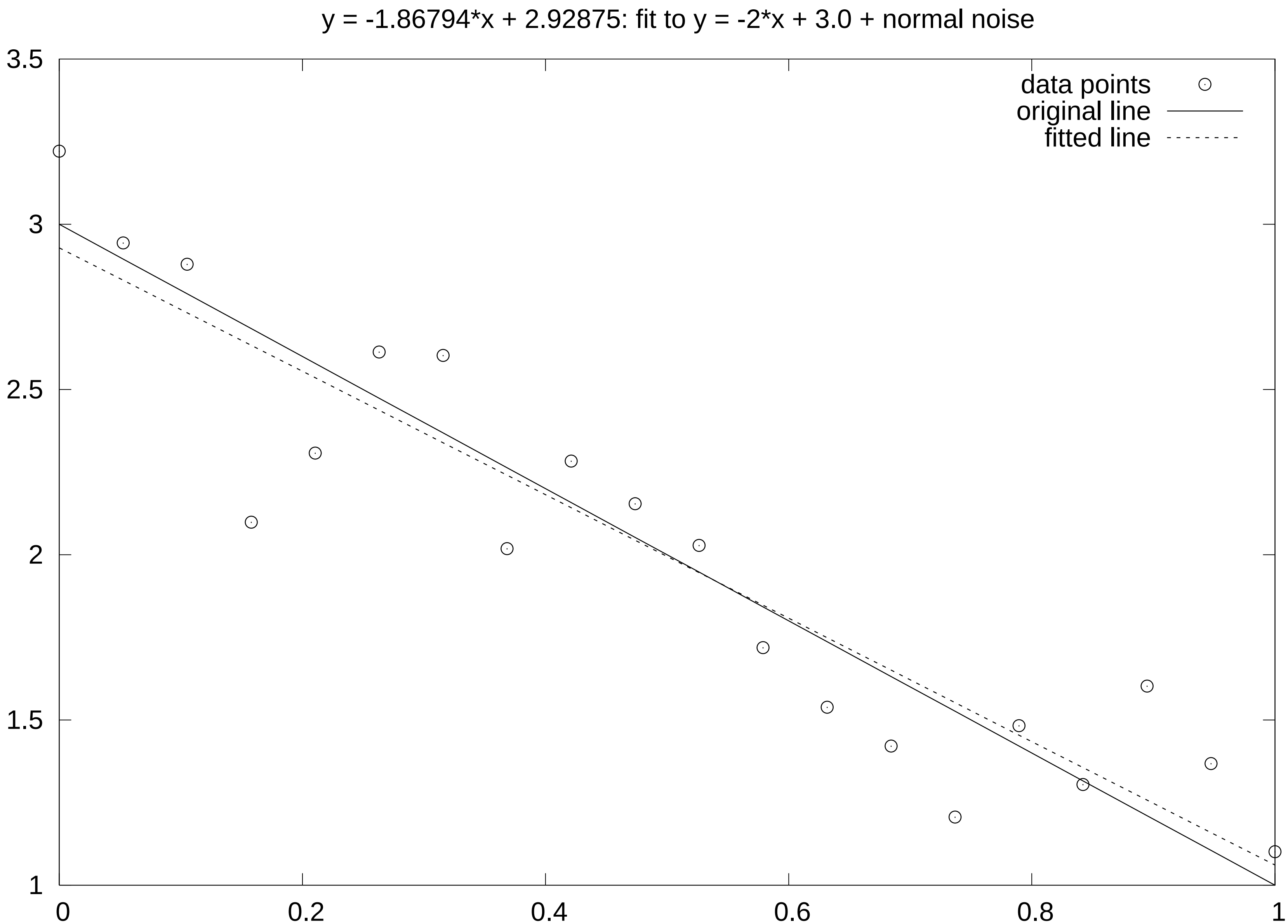
- NumPy enables efficient numerical computing in Python
- NumPy is a package of modules, which offers efficient arrays (contiguous storage) with associated array operations coded in C or Fortran
- There are three implementations of Numerical Python
  - Numeric from the mid 90s (still widely used)
  - numarray from about 2000
  - numpy from 2006
- We recommend to use numpy (by Travis Oliphant)

```
from numpy import *
```

A taste of NumPy: a least-squares procedure

```
x = linspace(0.0, 1.0, n)                   # coordinates
y_line = -2*x + 3
y = y_line + random.normal(0, 0.25, n)  # line with noise

# goal: fit a line to the data points x, y

# create and solve least squares system:
A = array([x, ones(n)])
A = A.transpose()

result = linalg.lstsq(A, y)
# result is a 4-tuple, the solution (a,b) is the 1st entry:
a, b = result[0]

plot(x, y, 'o',         # data points w/noise
     x, y_line, 'r',    # original line
     x, a*x + b, 'b')   # fitted lines
legend('data points', 'original line', 'fitted line')
hardcopy('myplot.png')
```

Resulting plot



Making arrays

```
>>> from numpy import *
>>> n = 4
>>> a = zeros(n)      # one-dim. array of length n
>>> print a
[ 0.  0.  0.  0.]
>>> a
array([ 0.,  0.,  0.,  0.])
>>> p = q = 2
>>> a = zeros((p,q,3))      # p*q*3 three-dim. array
>>> print a
[[[ 0.  0.  0.]
  [ 0.  0.  0.]]

 [[ 0.  0.  0.]
  [ 0.  0.  0.]]]
>>> a.shape                 # a's dimension
(2, 2, 3)
```

Making float, int, complex arrays

```
>>> a = zeros(3)
>>> print a.dtype # a's data type
float64
>>> a = zeros(3, int)
>>> print a
[0 0 0]
>>> print a.dtype
int32
>>> a = zeros(3, float32)    # single precision
>>> print a
[ 0.  0.  0.]
>>> print a.dtype
float32
>>> a = zeros(3, complex)
>>> a
array([ 0.+0.j,  0.+0.j,  0.+0.j])
>>> a.dtype
dtype('complex128')

>>> given an array a, make a new array of same dimension
>>> and data type:
>>> x = zeros(a.shape, a.dtype)
```

Array with a sequence of numbers

- `linspace(a, b, n)` generates `n` uniformly spaced coordinates, starting with `a` and ending with `b`

```
>>> x = linspace(-5, 5, 11)
>>> print x
[-5. -4. -3. -2. -1.  0.  1.  2.  3.  4.  5.]
```

- A special compact syntax is also available:

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

- `arange` works like `range` (`xrange`)

```
>>> x = arange(-5, 5, 1, float)
>>> print x  # upper limit 5 is not included!!
[-5. -4. -3. -2. -1.  0.  1.  2.  3.  4.]
```

Warning: arange is dangerous

- `arange`'s upper limit may or may not be included (due to round-off errors)
- Better to use a safer method: `seq(start, stop, increment)`

```
>>> from scitools.numpyutils import seq
>>> x = seq(-5, 5, 1)
>>> print x    # upper limit always included
[-5. -4. -3. -2. -1.  0.  1.  2.  3.  4.  5.]
```

- The package `scitools` is available at `http://code.google.com/p/scitools/`

Array construction from a Python list

- `array(list, [datatype])` generates an array from a list:

```
>>> pl = [0, 1.2, 4, -9.1, 5, 8]
>>> a = array(pl)
```

- The array elements are of the simplest possible type:

```
>>> z = array([1, 2, 3])
>>> print z                          # array of integers
[1 2 3]
>>> z = array([1, 2, 3], float)
>>> print z
[ 1.  2.  3.]
```

- A two-dim. array from two one-dim. lists:

```
>>> x = [0, 0.5, 1]; y = [-6.1, -2, 1.2]  # Python lists
>>> a = array([x, y])  # form array with x and y as rows
```

- From array to list: `alist = a.tolist()`

From “anything” to a NumPy array

- Given an object `a`,

  ```
  a = asarray(a)
  ```

  converts `a` to a NumPy array (if possible/necessary)

- Arrays can be ordered as in C (default) or Fortran:

  ```
  a = asarray(a, order='Fortran')
  isfortran(a)  # returns True if a's order is Fortran
  ```

- Use `asarray` to, e.g., allow flexible arguments in functions:

  ```
  def myfunc(some_sequence):
      a = asarray(some_sequence)
      return 3*a - 5

  myfunc([1,2,3])        # list argument
  myfunc((-1,1))         # tuple argument
  myfunc(zeros(10))      # array argument
  myfunc(-4.5)           # float argument
  myfunc(6)              # int argument
  ```

Changing array dimensions

```
>>> a = array([0, 1.2, 4, -9.1, 5, 8])
>>> a.shape = (2,3)        # turn a into a 2x3 matrix
>>> print a
[[ 0.   1.2  4. ]
 [-9.1  5.   8. ]]
>>> a.size
6
>>> a.shape = (a.size,)    # turn a into a vector of length 6 again
>>> a.shape
(6,)
>>> print a
[ 0.   1.2  4.  -9.1  5.   8. ]
>>> a = a.reshape(2,3)     # same effect as setting a.shape
>>> a.shape
(2, 3)
```

Array initialization from a Python function

```
>>> def myfunc(i, j):
...     return (i+1)*(j+4-i)
...
>>> # make 3x6 array where a[i,j] = myfunc(i,j):
>>> a = fromfunction(myfunc, (3,6))
>>> a
array([[  4.,   5.,   6.,   7.,   8.,   9.],
       [  6.,   8.,  10.,  12.,  14.,  16.],
       [  6.,   9.,  12.,  15.,  18.,  21.]])
```

Basic array indexing

Note: all integer indices in Python start at 0!

```
a = linspace(-1, 1, 6)
a[2:4] = -1        # set a[2] and a[3] equal to -1
a[-1]  = a[0]      # set last element equal to first one
a[:]   = 0         # set all elements of a equal to 0
a.fill(0)          # set all elements of a equal to 0

a.shape = (2,3)    # turn a into a 2x3 matrix
print a[0,1]       # print element (0,1)
a[i,j] = 10        # assignment to element (i,j)
a[i][j] = 10       # equivalent syntax (slower)
print a[:,k]       # print column with index k
print a[1,:]       # print second row
a[:,:] = 0         # set all elements of a equal to 0
```

More advanced array indexing

```
>>> a = linspace(0, 29, 30)
>>> a.shape = (5,6)
>>> a
array([[  0.,   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.,]])

>>> a[1:3,::2]    # a[i,j] for i=1,2 and j=0,2,4
array([[  6.,    8.,   10.],
       [ 12.,   14.,   16.]])

>>> a[::3,2::2]    # a[i,j] for i=0,3 and j=2,4
array([[  2.,    4.],
       [ 20.,   22.]])

>>> i = slice(None, None, 3);  j = slice(2, None, 2)
>>> a[i,j]
array([[  2.,    4.],
       [ 20.,   22.]])
```

Slices refer the array data

- With `a` as list, `a[:]` makes a copy of the data
- With `a` as array, `a[:]` is a reference to the data

```
>>> b = a[2,:]         # extract 2nd row of a
>>> print a[2,0]
12.0
>>> b[0] = 2
>>> print a[2,0]
2.0                    # change in b is reflected in a!
```

- Take a copy to avoid referencing via slices:

```
>>> b = a[2,:].copy()
>>> print a[2,0]
12.0
>>> b[0] = 2        # b and a are two different arrays now
>>> print a[2,0]
12.0                # a is not affected by change in b
```

Loops over arrays (1)

- Standard loop over each element:

```
for i in xrange(a.shape[0]):
    for j in xrange(a.shape[1]):
        a[i,j] = (i+1)*(j+1)*(j+2)
        print 'a[%d,%d]=%g ' % (i,j,a[i,j]),
    print  # newline after each row
```

- A standard for loop iterates over the first index:

```
>>> print a
[[  2.   6.  12.]
 [  4.  12.  24.]]
>>> for e in a:
...     print e
...
[  2.   6.  12.]
[  4.  12.  24.]
```

Loops over arrays (2)

- View array as one-dimensional and iterate over all elements:

  ```
  for e in a.ravel():
      print e
  ```

  Use `ravel()` only when reading elements, for assigning it is better to use `shape` or `reshape` first!

- For loop over all index tuples and values:

  ```
  >>> for index, value in ndenumerate(a):
  ...     print index, value
  ...
  (0, 0) 2.0
  (0, 1) 6.0
  (0, 2) 12.0
  (1, 0) 4.0
  (1, 1) 12.0
  (1, 2) 24.0
  ```

Array computations

- Arithmetic operations can be used with arrays:

  ```
  b = 3*a - 1    # a is array, b becomes array
  ```

  1) compute `t1 = 3*a`, 2) compute `t2= t1 - 1`, 3) set `b = t2`

- Array operations are much faster than element-wise operations:

  ```
  >>> import time  # module for measuring CPU time
  >>> a = linspace(0, 1, 1E+07)  # create some array
  >>> t0 = time.clock()
  >>> b = 3*a -1
  >>> t1 = time.clock()   # t1-t0 is the CPU time of 3*a-1

  >>> for i in xrange(a.size): b[i] = 3*a[i] - 1
  >>> t2 = time.clock()
  >>> print '3*a-1: %g sec, loop: %g sec' % (t1-t0, t2-t1)
  3*a-1: 2.09 sec, loop: 31.27 sec
  ```

Standard math functions can take array arguments

```
# let b be an array

c = sin(b)
c = arcsin(c)
c = sinh(b)
# same functions for the cos and tan families

c = b**2.5  # power function
c = log(b)
c = exp(b)
c = sqrt(b)
```

Other useful array operations

```
# a is an array

a.clip(min=3, max=12)   # clip elements
a.mean(); mean(a)       # mean value
a.var();  var(a)        # variance
a.std();  std(a)        # standard deviation
median(a)
cov(x,y)                # covariance
trapz(a)                # Trapezoidal integration
diff(a)                 # finite differences (da/dx)

# more Matlab-like functions:
corrcoeff, cumprod, diag, eig, eye, fliplr, flipud, max, min,
prod, ptp, rot90, squeeze, sum, svd, tri, tril, triu
```

More useful array methods and attributes

```
>>> a = zeros(4) + 3
>>> a
array([ 3.,  3.,  3.,  3.])  # float data
>>> a.item(2)                # more efficient than a[2]
3.0
>>> a.itemset(3,-4.5)        # more efficient than a[3]=-4.5
>>> a
array([ 3. ,  3. ,  3. , -4.5])
>>> a.shape = (2,2)
>>> a
array([[ 3. ,  3. ],
       [ 3. , -4.5]])
>>> a.ravel()                # from multi-dim to one-dim
array([ 3. ,  3. ,  3. , -4.5])
>>> a.ndim                   # no of dimensions
2
>>> len(a.shape)             # no of dimensions
2
>>> rank(a)                  # no of dimensions
2
>>> a.size                   # total no of elements
4
>>> b = a.astype(int)        # change data type
>>> b
array([3, 3, 3, 3])
```

Modules for curve plotting and 2D/3D visualization

- Matplotlib (curve plotting, 2D scalar and vector fields)
- PyX (PostScript/TeX-like drawing)
- Interface to Gnuplot
- Interface to Vtk
- Interface to OpenDX
- Interface to IDL
- Interface to Grace
- Interface to Matlab
- Interface to R
- Interface to Blender

Curve plotting with Easyviz

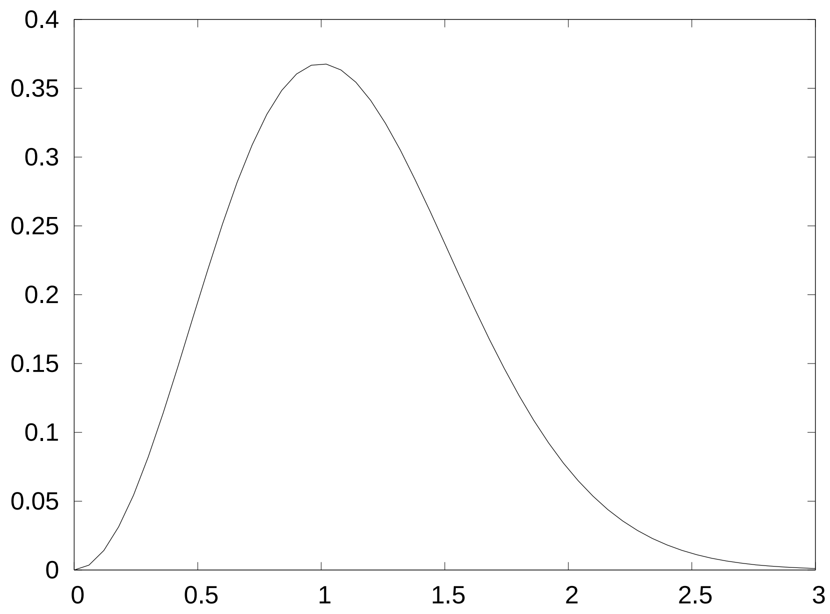
- Easyviz is a light-weight interface to many plotting packages, using a Matlab-like syntax
- Goal: write your program using Easyviz (“Matlab”) syntax and postpone your choice of plotting package
- Note: some powerful plotting packages (Vtk, R, matplotlib, ...) may be troublesome to install, while Gnuplot is easily installed on all platforms
- Easyviz supports (only) the most common plotting commands
- Easyviz is part of SciTools (Simula development)

  ```
  from scitools.all import *
  ```

  (imports all of `numpy`, all of `easyviz`, plus `scitools`)

Basic Easyviz example

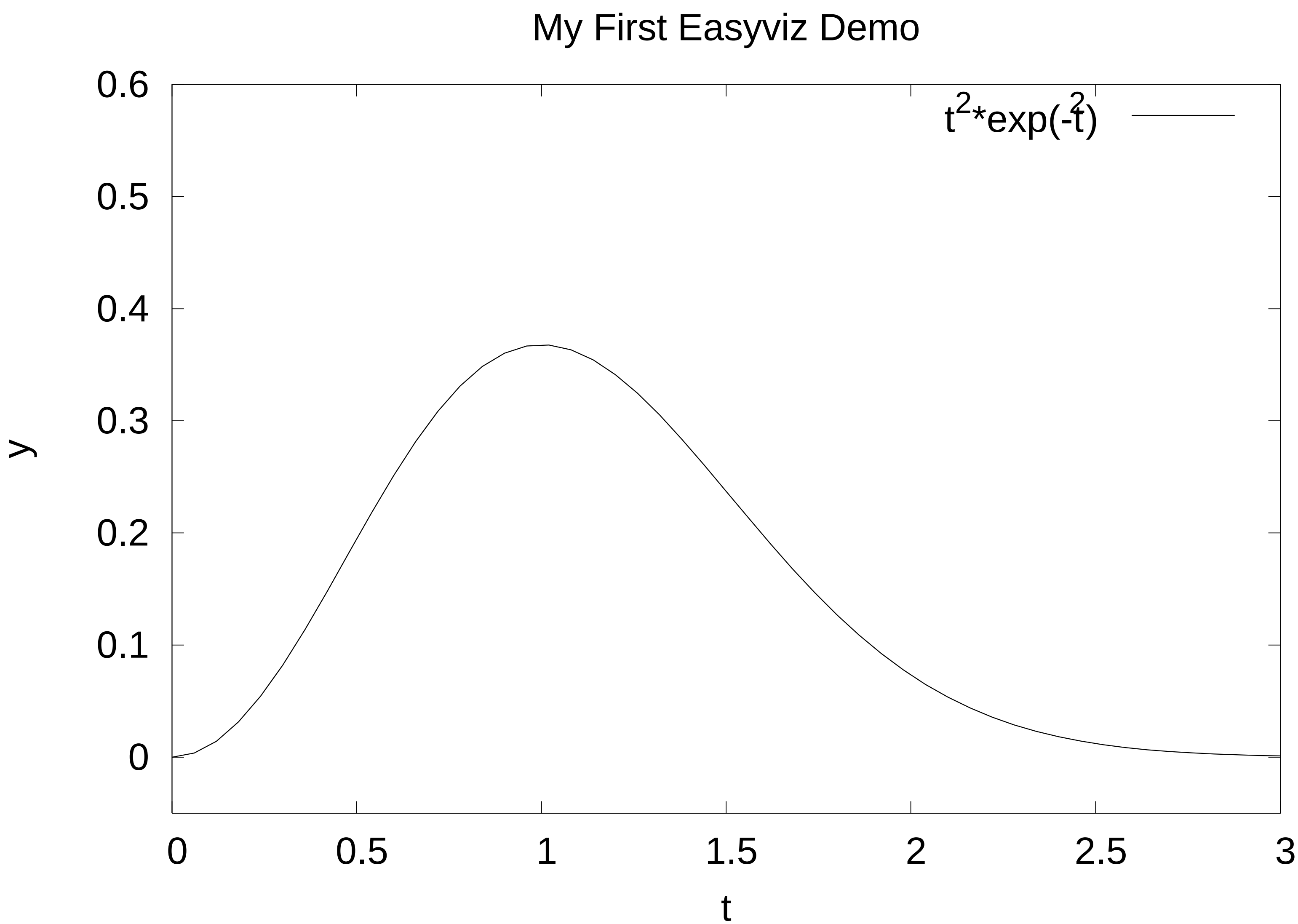
```
from scitools.all import *   # import numpy and plotting
t = linspace(0, 3, 51)       # 51 points between 0 and 3
y = t**2*exp(-t**2)          # vectorized expression
plot(t, y)
hardcopy('tmp1.eps')  # make PostScript image for reports
hardcopy('tmp1.png')  # make PNG image for web pages
```



Decorating the plot

```
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')

# or
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',
     hardcopy='tmp1.eps',
     show=True)   # display on the screen (default)
```

The resulting plot

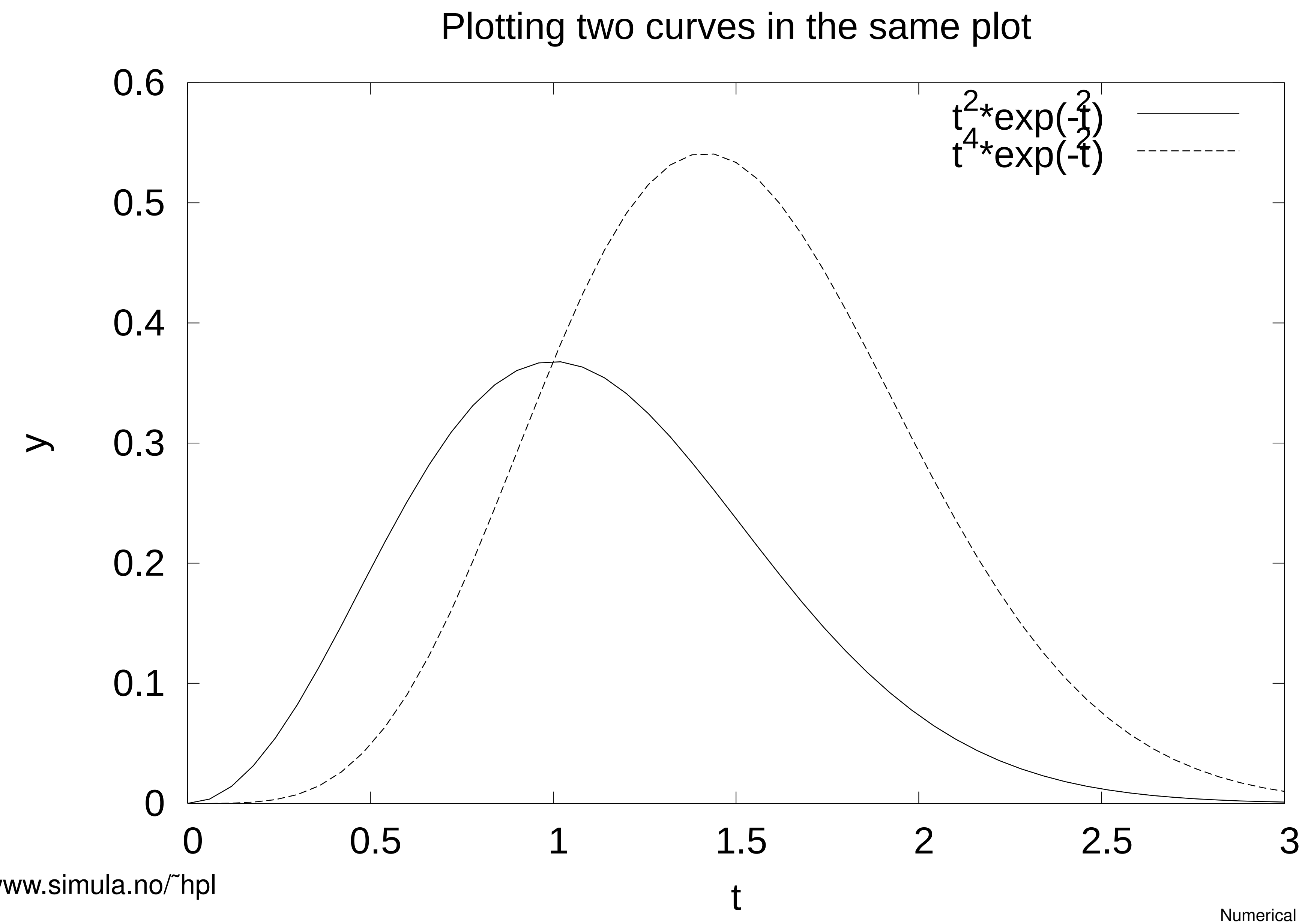


Plotting several curves in one plot

Compare $f_1(t) = t^2 e^{-t^2}$ and $f_2(t) = t^4 e^{-t^2}$ for $t \in [0, 3]$

```
from scitools.all import *   # for curve plotting

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')    # 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')
hardcopy('tmp2.eps')
```

The resulting plot



Example: plot a function given on the command line

- Task: plot (e.g.) $f(x) = e^{-0.2x}\sin(2\pi x)$ for $x \in [0, 4\pi]$
- Specify $f(x)$ and x interval as text on the command line:

```
Unix/DOS> python plotf.py "exp(-0.2*x)*sin(2*pi*x)" 0 4*pi
```

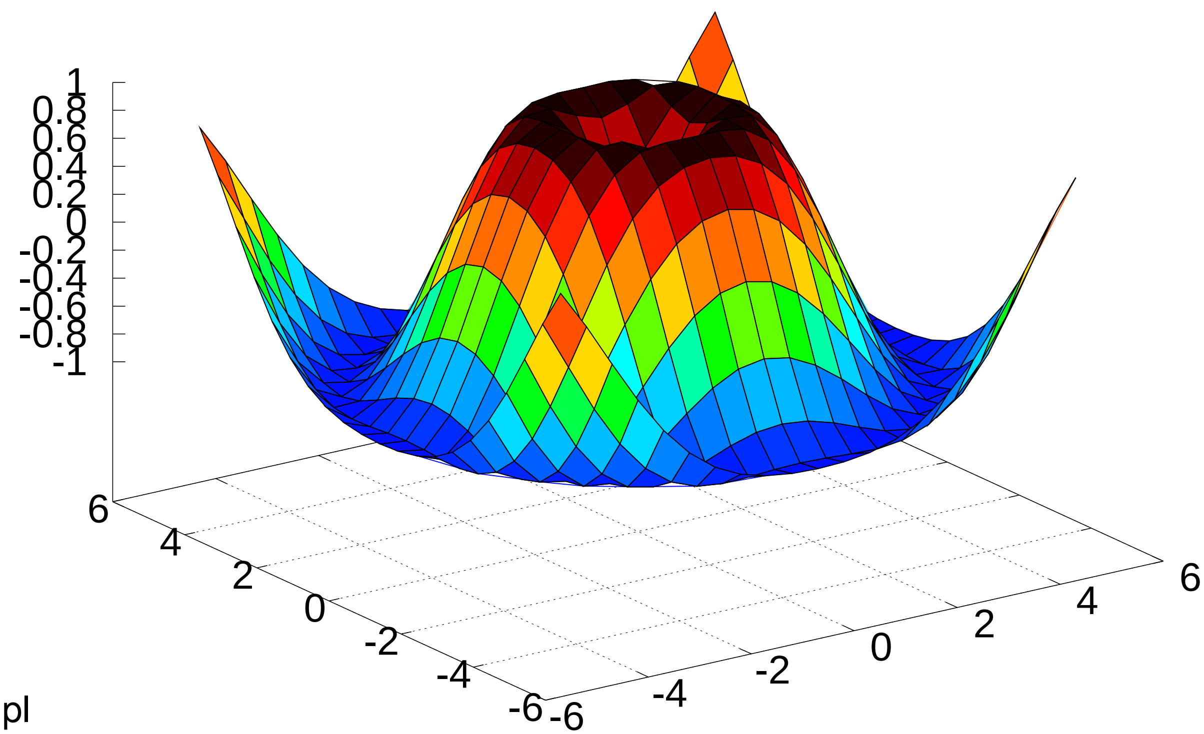
- Program:

```
from scitools.all import *
formula = sys.argv[1]
xmin = eval(sys.argv[2])
xmax = eval(sys.argv[3])

x = linspace(xmin, xmax, 101)
y = eval(formula)
plot(x, y, title=formula)
```

- Thanks to `eval`, input (text) with correct Python syntax can be turned to running code on the fly

Plotting 2D scalar fields

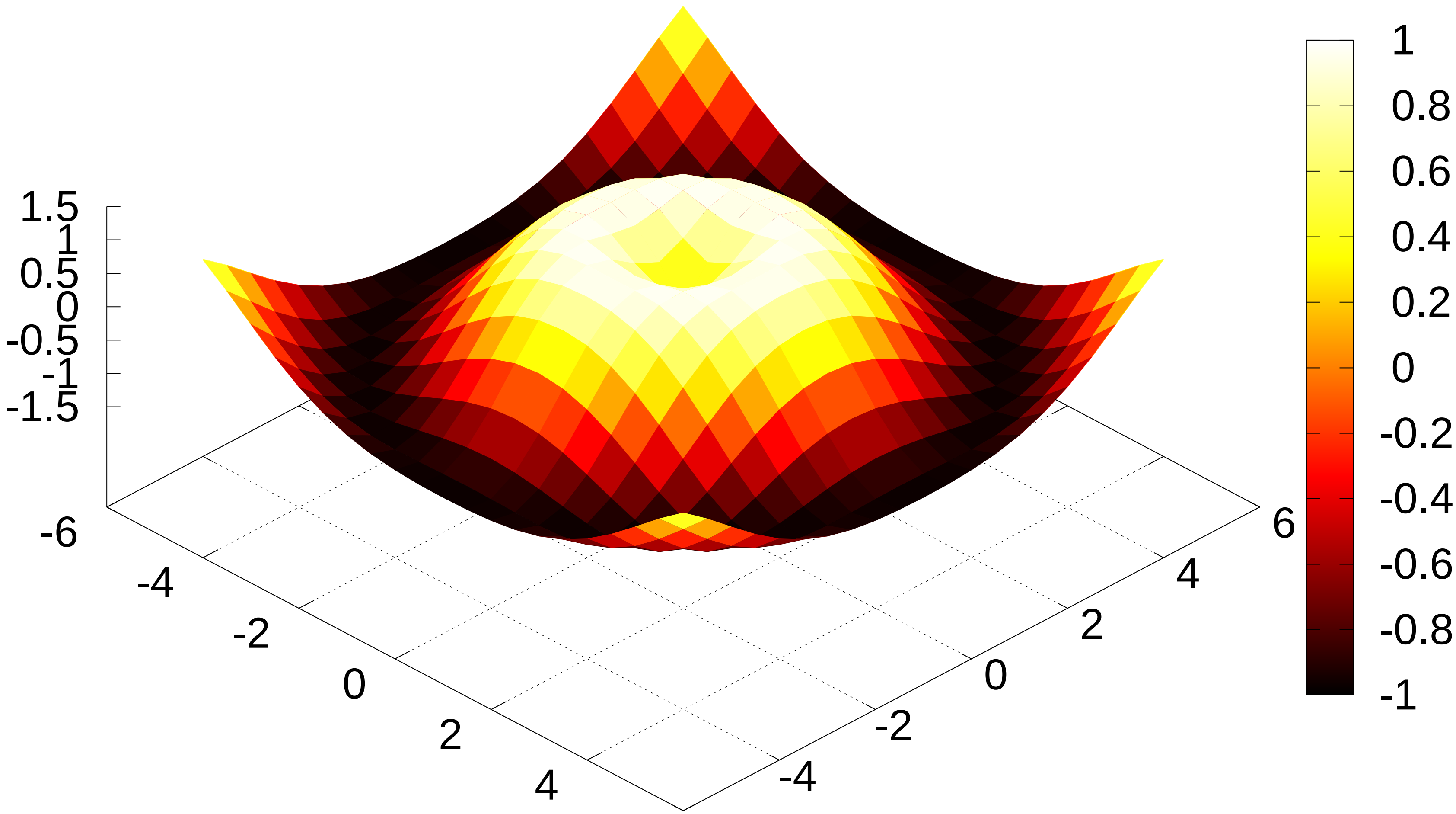
```
from scitools.all import *

x = y = linspace(-5, 5, 21)
xv, yv = ndgrid(x, y)
values = sin(sqrt(xv**2 + yv**2))
surf(xv, yv, values)
```



Adding plot features

```
# Matlab style commands:
setp(interactive=False)
surf(xv, yv, values)
shading('flat')
colorbar()
colormap(hot())
axis([-6,6,-6,6,-1.5,1.5])
view(35,45)
show()

# Optional Easyviz (Pythonic) short cut:
surf(xv, yv, values,
     shading='flat',
     colorbar='on',
     colormap=hot(),
     axis=[-6,6,-6,6,-1.5,1.5],
     view=[35,45])
```

The resulting plot



Other commands for visualizing 2D scalar fields

- `contour` (standard contours)), `contourf` (filled contours), `contour3` (elevated contours)
- `mesh` (elevated mesh), `meshc` (elevated mesh with contours in the xy plane)
- `surf` (colored surface), `surfc` (colored surface with contours in the xy plane)
- `pcolor` (colored cells in a 2D mesh)

Commands for visualizing 3D fields

Scalar fields:

- `isosurface`
- `slice_` (colors in slice plane), `contourslice` (contours in slice plane)

Vector fields:

- `quiver3` (arrows), (`quiver` for 2D vector fields)
- `streamline`, `streamtube`, `streamribbon` (flow sheets)

More info about Easyviz

- A plain text version of the Easyviz manual:

```
pydoc scitools.easyviz
```

- The HTML version:

```
http://code.google.com/p/scitools/wiki/EasyvizDocumentation
```

- Download SciTools (incl. Easyviz):

```
http://code.google.com/p/scitools/
```

Python optimization

Contents

- Timing and profiling.
- Simple Python tricks.
- Vectorization and mixed-language programming.

Optimization of C, C++, and Fortran

- Compilers do a good job for C, C++, and Fortran.
- The type system makes agressive optimization possible.
- Examples: code inlining, loop unrolling, and memory prefetching.

Python optimization

- No compiler.
- No type declaration of variables.
- No inlining and no loop unrolling.
- Probably inefficient in Python:

```
def f(a, b):
    return a + b
```

Manual timing

- Use `time.time()`.
- Simple statements should be placed in a loop.
- Make sure constant machine load.
- Run the tests several times, choose the fastest.

The `timeit` module (1)

- Usage:

```
import timeit
timer =
timeit.Timer(stmt="a+=1",setup="a=0")
time = timer.timeit(number=10000) #or
times = timer.repeat(repeat=5,
number=10000)
```

The `timeit` module (2)

- Isolates the global namespace.
- Automatically wraps the code in a for–loop.
- Users can provide their own timer (callback).
- Time a user defined function:
  ```
  timer = timeit.Timer(stmt="myfunc()",
  setup="from __main__ import my_func")
  ```

Profiling modules

- Prior to code optimization, hotspots and bottlenecks must be located.
  "First make it work. Then make it right. Then make it fast."
  - Kent Beck
- Two main modules: `profile` and `cProfile` (`hotshot` is no longer maintained).
- `profile` works for all Python versions.
- `cProfile` introduced in Python version 2.5.

The `profile` module (1)

- As a script: `profile.py script.py`
- As a module:

```
import profile
pr = profile.Profile()
res = pr.run("function()", "filename")
res.print_stats()
```

- Profile data saved to "filename" can be viewed with the `pstats` module.

The `profile` module (2)

- `profile.calibrate(number)` finds the profiling overhead.
- Remove profiling overhead:
  `pr = profile.Profile(bias=overhead)`
- Profile a single function call:

```
pr = profile.Profile()
pr.runcall(func, *args, **kwargs)
```

The `cProfile` module (recommended)

- Similar to `profile`, but mostly implemented in C.
- Smaller performance impact than `profile`.
- Useage:

  ```
  import cProfile
  cProfile.run('foo()', 'fooprof')
  ```

  or to profile a script:

  ```
  python -m cProfile my_script.py
  ```

The `pstats` module

- There are many ways to view profiling data.
- The module `pstats` provides the class `Stats` for creating profiling reports:

```
import pstats
data = pstats.Stats("fooprof")
data.print_stats()
```

- The method `sort_stats(key, *keys)` is used to sort future output.
- Common used keys: `'calls'`, `'cumulative'`, `'time'`.

Pure Python performance tips

- Place references to functions in the local namespace.

```
from math import *
def f(x):
    for i in xrange(len(x)):
        x[i] = sin(x[i]) # Slow
    return x

def g(x):
    loc_sin = sin # Local reference
    for i in xrange(len(x)):
        x[i] = loc_sin(x[i]) # Faster
    return x
```

- Reason: Local namespace is searched first.

More local references

- Local references to instance methods of global objects are even more important, as we need only one dictionary look–up to find the method instead of three (local, global, instance–dictionary).

```
class Dummy(object):
    def f(self): pass

d = Dummy()

def f():
    loc_f=d.f
    for i in xrange(10000): loc_f()
```

- Calling `loc_f()` instead of `d.f()` is 40% faster in this example.

Exceptions should never happen

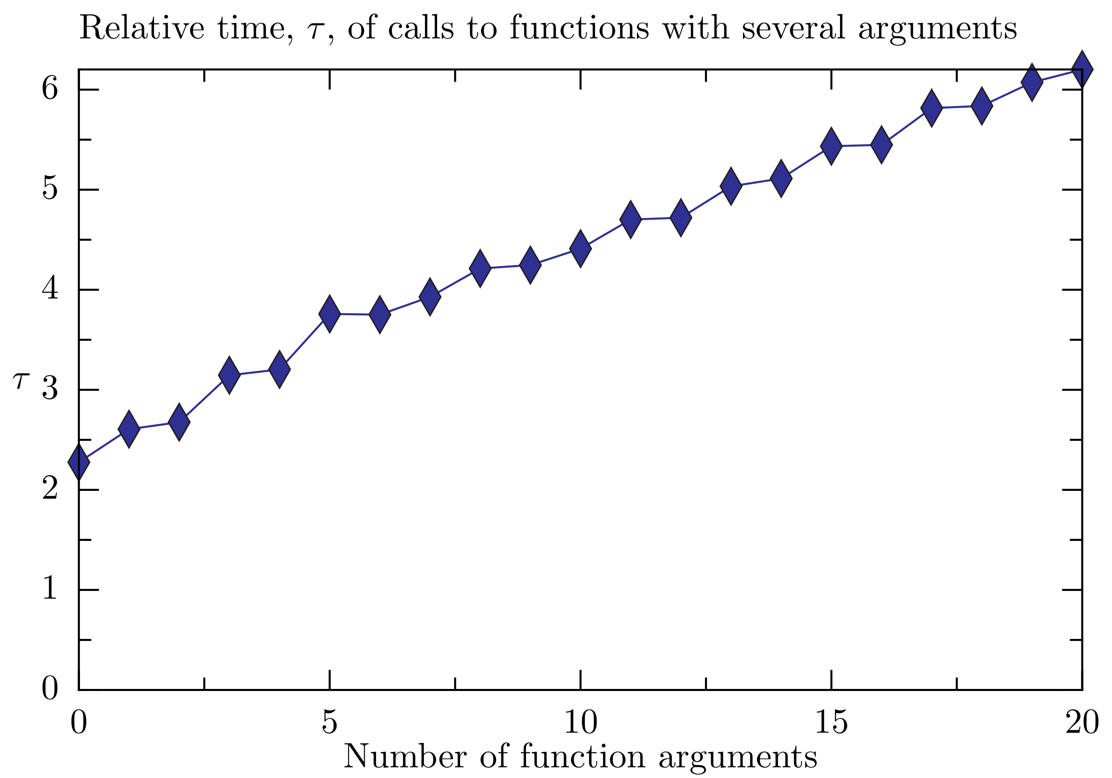
- Use `if/else` instead of `try/except`
- Example:

```
x = 0
try: 1.0/x
except: 0

if not (x==0): 1.0/x
else: 0
```

- `if/else` is more than 20 times faster.

Function calls

- The time of calling a function grows linearly with the number of arguments:



Numerical Python

- Vectorized computations are fast:

```
import numpy
x = numpy.arange(-1,1,0.01)
y = numpy.sin(x)
```

```
import math # Scalar functions
y = numpy.zeros(len(x))
for i in xrange(len(x)):
    y[i] = math.sin(x[i])
```

- The speedup is a factor of 20.

Resizing arrays

- The `resize` method of arrays is very slow.
- Increasing the array size by one in a loop is about 300-350 times slower than appending elements to a Python list.
- Best approach; allocate the memory once, and assign values later.

Conclusions

- Python scripts can often be heavily optimized.
- The results given here may vary on different architectures and Python versions
- Be extremely careful about the `from numpy import *`. For scalar arguments, functions from the `math` module are much faster than the corresponding `numpy` functions.
- Vectorized computations can achieve similar efficiency as optimized compiled language code.
- Time-critical operations that cannot be vectorized must be ported to a compiled language.