Ch.5: Array computing and curve plotting (Part 1)

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Plan for week 38

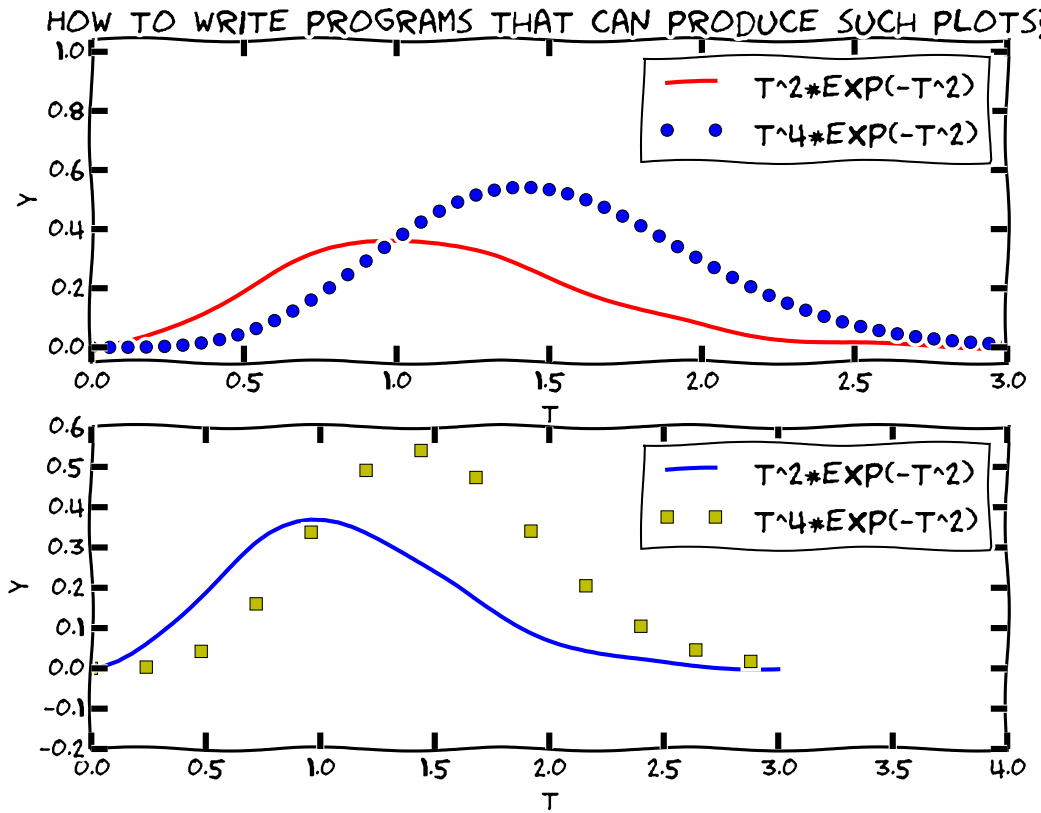
Tuesday 18 september

- Live programming of ex 4.4, 4.5, 4.6, 4.7
- Intro to NumPy arrays and plotting

Thursday 22 september

- Live programming of ex 5.7, 5.9, 5.10, 5.11, 5.13
- Plotting with `matplotlib`
- (Making movies and animations from plots)

Goal: learn to visualize functions



We need to learn about a new object: array

- Curves $y = f(x)$ are visualized by drawing straight lines between points along the curve
- Need to store the coordinates of the points along the curve in lists or *arrays* `x` and `y`
- Arrays $\approx$ 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!

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

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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

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

- 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:

```
>>> def f(x):
...     return x**3
...
>>> n = 5                    # no of points
>>> dx = 1.0/(n-1)           # x spacing 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)]
```

Turn lists into Numerical Python (NumPy) arrays:

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

Make arrays directly (instead of lists)

The pro drops lists and makes NumPy arrays directly:

```
>>> n = 5                          # number of points
>>> x = np.linspace(0, 1, n) # n points in [0, 1]
>>> y = np.zeros(n)                # n zeros (float data type)
>>> for i in range(n):
...     y[i] = f(x[i])
...
```

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 range(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.

Vectorization gives:

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

A function f(x) written for a number x usually works for array x too

```
from numpy import sin, exp, linspace

def f(x):
    return x**3 + sin(x)*exp(-3*x)

x = 1.2                          # float object
y = f(x)                         # y is float

x = linspace(0, 3, 10001)        # 10000 intervals in [0,3]
y = f(x)                         # y is array
```

Note: math is for numbers and numpy for arrays

```
>>> import math, numpy
>>> x = numpy.linspace(0, 1, 11)
>>> math.sin(x[3])
0.2955202066613396
>>> math.sin(x)
...
TypeError: only length-1 arrays can be converted to Python scalars
>>> numpy.sin(x)
array([ 0.        ,  0.09983,  0.19866,  0.29552,  0.38941,
        0.47942,  0.56464,  0.64421,  0.71735,  0.78332,
        0.84147])
```

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)

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Small quiz:

What is output from the following code? Why?

```
import numpy as np

l = [0,0.25,0.5,0.75,1]
a = np.array(l)

print(l*2)
print(a*2)
```

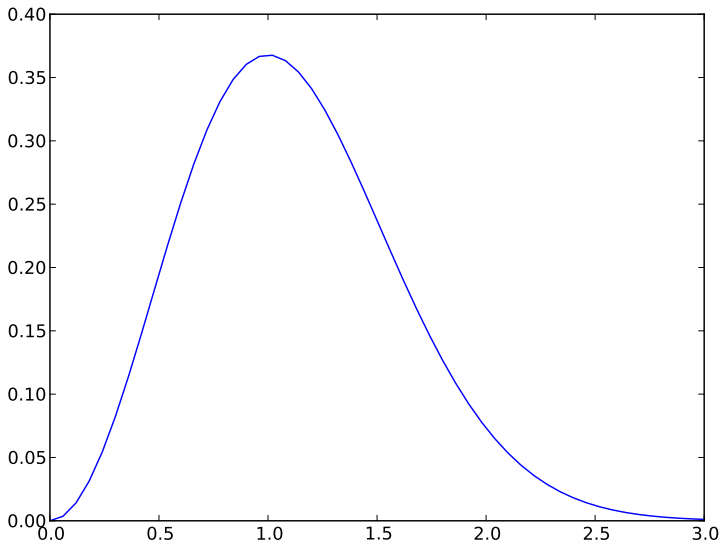
Plotting the curve of a function: the very basics

Plot the curve of $y(t) = t^2 e^{-t^2}$:

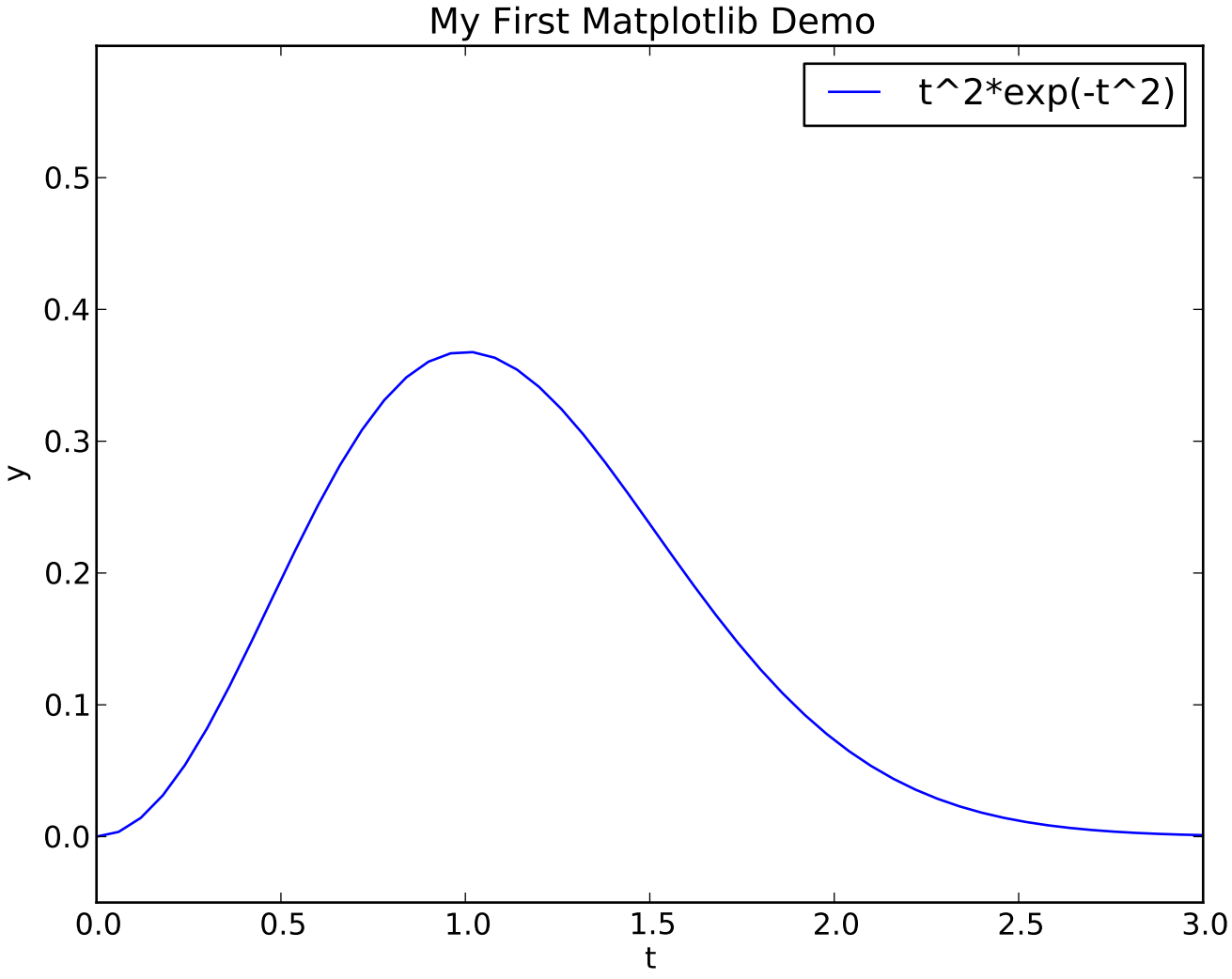
```
from matplotlib.pyplot import *  # import and plotting
from numpy import *

# 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 PNG image for web pages
show()
```



A plot should have labels on axis and a title



The code that makes the last plot

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

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,label="t^2*exp(-t^2)")

xlabel('t')                # label on the x axis
ylabel('y')                # label on the y axix
legend()                   # mark the curve
axis([0, 3, -0.05, 0.6])   # [tmin, tmax, ymin, ymax]
title('My First Matplotlib Demo')
show()
```

Plotting several curves in one plot

Plot $t^2e^{-t^2}$ and $t^4e^{-t^2}$ in the same plot:

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

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

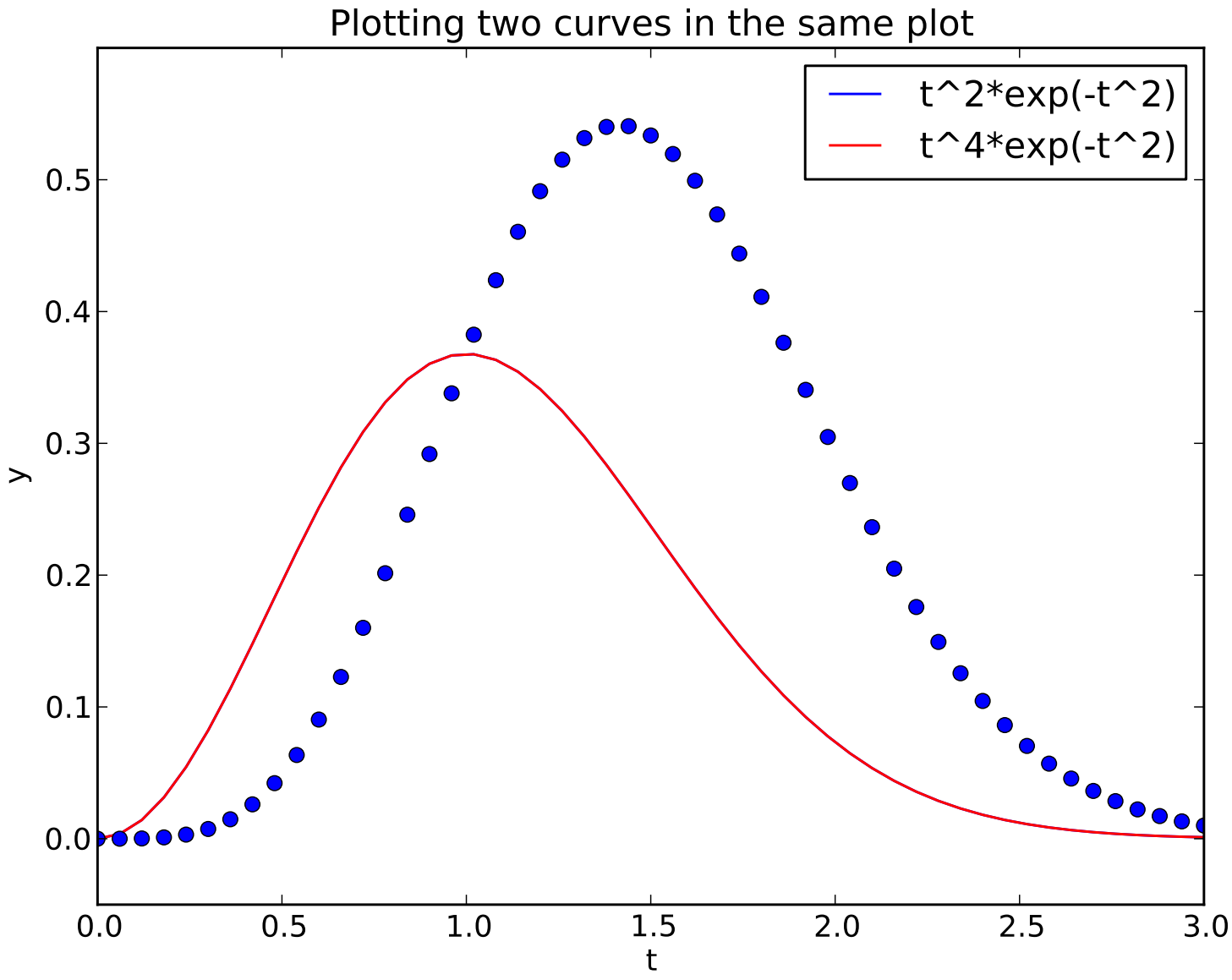
def f2(t):
    return t**2*f1(t)

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

plot(t, y1,  'r-', label = 't^2*exp(-t^2)')
plot(t, y2, 'bo', label = 't^4*exp(-t^2)')

xlabel('t')
ylabel('y')
legend()
title('Plotting two curves in the same plot')
savefig('tmp2.png')
show()
```

The resulting plot with two curves



Controlling line styles

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 (-)

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 matplotlib.pyplot
```

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))
```

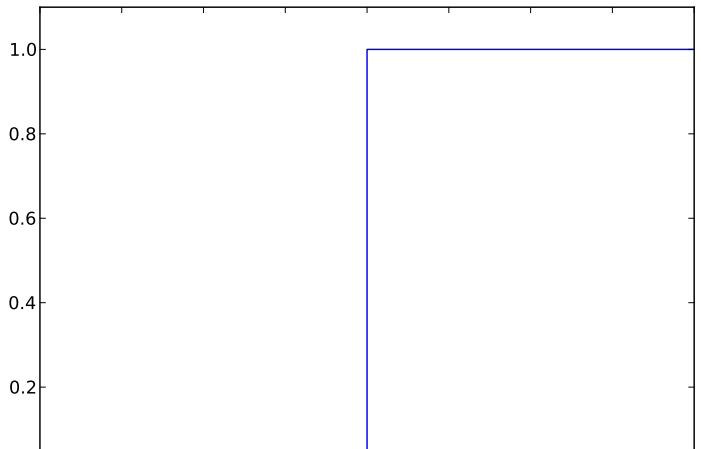
Let's try to plot a discontinuous function

The Heaviside function is frequently used in science and engineering:

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

Python implementation:

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



Plotting the Heaviside function: first try

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

`if x < 0` does not work if `x` is array

Remedy 1: use a loop over `x` values

```
def H_loop(x):
    r = zeros(len(x))  # or r = x.copy()
    for i in range(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

`if x < 0` does not work if `x` is array

Remedy 2: use `vectorize`

```
from numpy import vectorize

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

Downside: The resulting function is as slow as Remedy 1

`if x < 0` does not work if `x` is array

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):
    x1 = <expression1>
    x2 = <expression2>
    r = np.where(condition, x1, x2)
    return r
```

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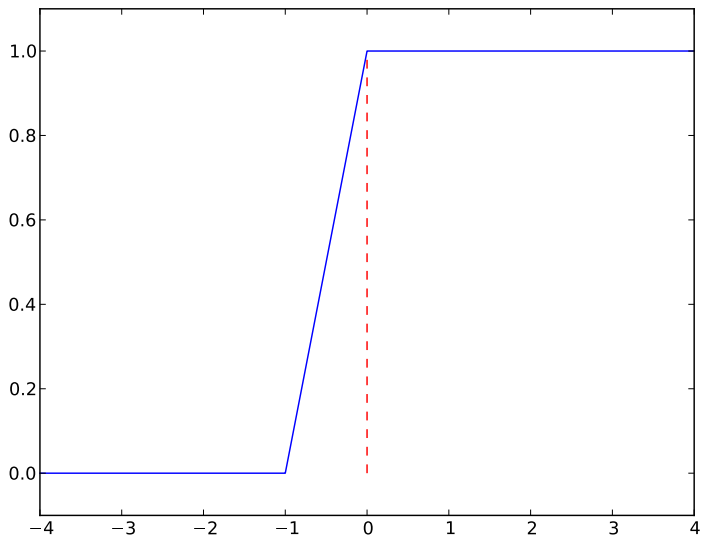
    x2 = <expression2>
    r = np.where(condition, x1, x2)
    return r
```

Back to plotting the Heaviside function

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])
```



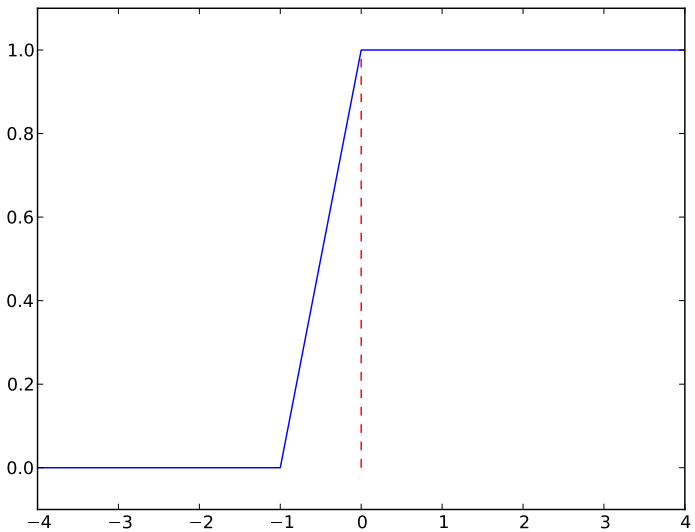
How to make the function look discontinuous in the plot?

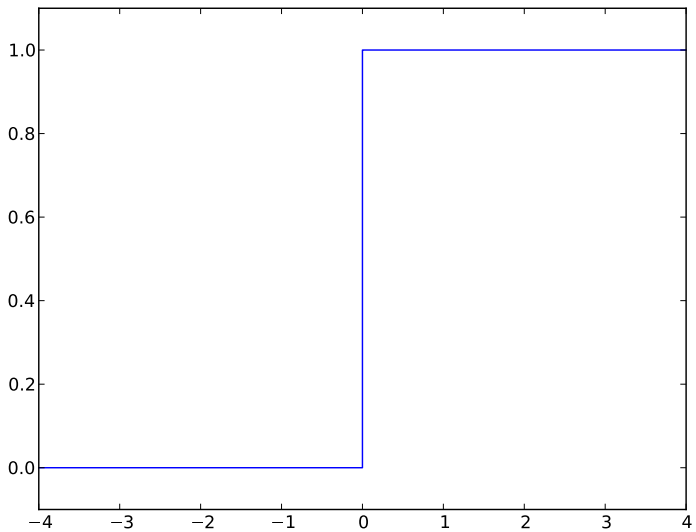
- Newbie: use a lot of x points; the curve gets steeper
- Pro: plot just two horizontal line segments
  one from $x = -10$ to $x = 0$, $y = 0$; and one from $x = 0$ to $x = 10$, $y = 1$

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

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

The final plot of the discontinuous Heaviside function





Removing the vertical jump from the plot

Question

Some will argue and say that at high school they would draw $H(x)$ as two horizontal lines *without* the vertical line at $x = 0$, illustrating the jump. How can we plot such a curve?

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.

Solution

Complete program:

```
from numpy import *
from matplotlib.pyplot 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)
show()
```