

Ecosystem

Modules

- Different way for import
 - Full package in it's own namespace:

```
import package
package.function()
# or
import package as pkg
pkg.function()
```

- Only function in package:

```
from package import function
function()
# or
from package import function as func
func()
```

- Full package in the current namespace: **TO BE AVOIDED**

```
from package import *
function()
```

Standard library

- builtins : automatically imported, contains basis (int, print(), ...)
- sys et os : two common modules for read and manage code's environment
- shutil : file managment (copy, move, ...)
- math / cmath : classic mathematical functions (real / complex)
- copy : particulary deepcopy
- pathlib : dedicated to pathfile managment
(directory / file better than directory + "/" + fichier)
- time
- ...

Your modules

- `import file` in order to use content of `file.py`
- if subfolders:
 - `__init__.py` mandatory in dir (may be empty)
 - `import dir.file` in order to use content of `dir/file.py`
- import involve execution!

```
if __name__ == '__main__':  
    # do stuff  
    ...
```

- can be imported:
 - each module in `sys.path` (feeded par `PYTHONPATH`)
 - each submodule (with `spam.egg`; `import spam` then `egg` in the directory `spam`)

It is useless to import a module multiple times (but it does not harm either)

In [1]:

```
from sys import path  
print(path)
```

```
['', '/usr/lib/python35.zip', '/usr/lib/python3.5', '/usr/lib/pytho  
n3.5/plat-x86_64-linux-gnu', '/usr/lib/python3.5/lib-dynload', '/Da  
ta/WORK/Formations/Python/formation_python/venv/lib/python3.5/site-  
packages', '/opt/local/jupyter-fortran-kernel', '/Data/WORK/Formati  
ons/Python/formation_python/venv/lib/python3.5/site-packages/IPytho  
n/extensions', '/home/pouxa/.ipython']
```

How to install external packages

- Windows
 - `conda install package`
 - `pip install package`
- Linux et Mac
 - `pip install --user package`

Numpy

[Reference \(https://docs.scipy.org/doc/numpy/reference/\)](https://docs.scipy.org/doc/numpy/reference/)

[Comparison from matlab \(http://mathesaurus.sourceforge.net/matlab-python-xref.pdf\)](http://mathesaurus.sourceforge.net/matlab-python-xref.pdf)

- `dtype` : numerical precision (double by default)
- `ndarray` : an array of a unique `dtype` unique **much faster** than the python lists
- `shape`
- **mutable**

- same indexing and slicing as with lists, plus:
 - a list of integers per dimensions
 - an array of index
 - an array of boolean (mask)
- creation :
 - empty : fast allocation but without initialization
 - zeros, zeros_like, ones, ones_like : allocation and initialization with 0 or 1
 - arange(start, end, step)
 - linspace(start, end, nb of points)
 - meshgrid : mesh
- matrix product : @
- **A lot** of packages use this data structure
- Some usefull functions
 - linalg.eigvals : eigen values
 - linalg.det : determinant
 - linalg.solve : solve $Ax = b$
 - linalg.inv : inverse a matrix
 - sort : sort
 - where : index where a mask is True
 - median, average, std, var : classic statistical tools
 - cov : covariant matrix
 - histogram : histogram

scipy

[Reference \(https://docs.scipy.org/doc/scipy/reference/\)](https://docs.scipy.org/doc/scipy/reference/)

- Many usefull constants
- **A lot** of usefull functions
 - fft, dct, dst : fourrier transform
 - quad, simps, odr : integration
 - solve_ivp, solve_bvp : ODE solver
 - griddata, make_interp_spline : interpolation
 - solve, inv, det, eigvals : linalg variant
 - lu, svd : more linalg
 - convolve, correlate, gaussian_filter, spline_filter : filters
 - binary_closing, binary_dilatation, binary_erosion : morphology
 - minimize, leastsq, root, fsolve : optimization and zeros finding
 - find_peaks_cwt, spectrogram : signal processing
 - lu, csr : sparse matrices
 - bicg, gmres, splu : sparse linalg
 - shortest_path : graph computation
 - KDTree, Delaunay, spatial computation
 - gauss, laplace, uniform, binom : random distributions
 - describe, bayes_mvs : more statistics
 - airy, jv, erf, fresnel : classical functions

Matplotlib

Gallery (<https://matplotlib.org/gallery/index.html>)

- Almost anything you need to visualize something
 - 1d / 2d / 3d
 - fixed or animated
 - static or interactive (but static is easier)
- Very close to the matlab syntax (too close ?)
- A lot of functionalities (too much ?)
- Might be slow (does not always replace paraview / visit)

Some exemples

In [2]:

```
import numpy as np

def f(t):
    """A simple function"""
    return np.exp(-t) * np.cos(2 * np.pi * t)

# Some time steps
t = np.arange(0.0, 5.0, 0.1)

# apply f() on all the values in t, and name the result y
y = f(t)

print("Numpy arrays are capable of some basic computation:")
print("{:6} = {:5.2f}\n" * 3).format("y min", y.min(),
                                     "y mean", y.mean(),
                                     "y max", y.max()))
```

Numpy arrays are capable of some basic computation:

```
y min = -0.61
y mean = 0.02
y max = 1.00
```

In [3]:

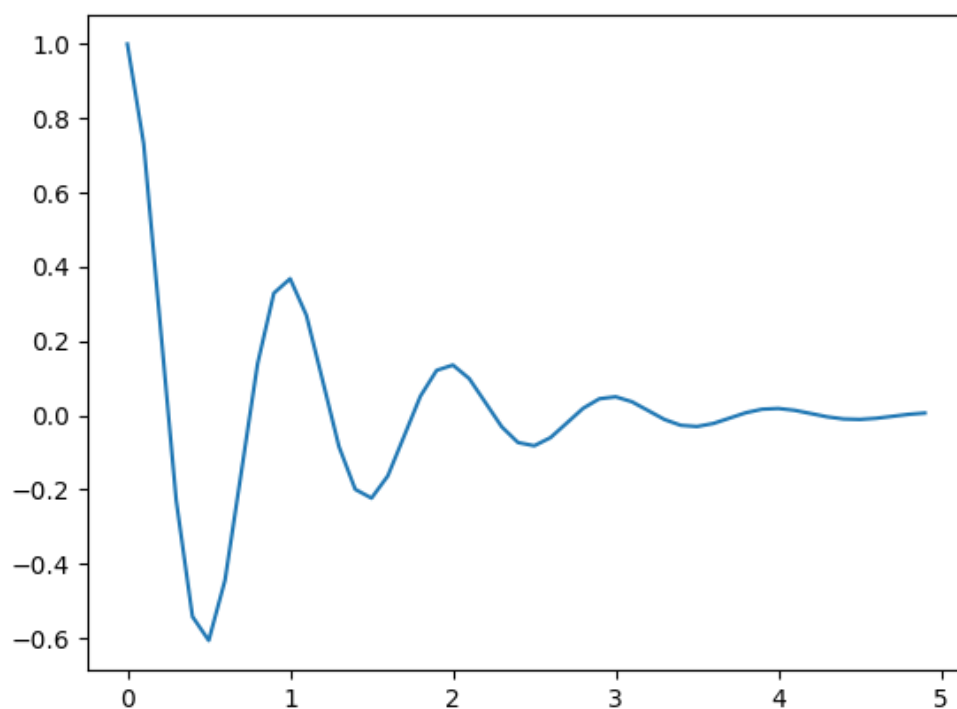
```
print("Or we can use numpy's functions on those arrays (see reference):")
print("{:6} = {:5.2f}\n" * 3).format("y min", np.min(y),
                                     "y mean", np.mean(y),
                                     "y max", np.max(y))
```

Or we can use numpy's functions on those arrays (see reference):

```
y min = -0.61
y mean = 0.02
y max = 1.00
```

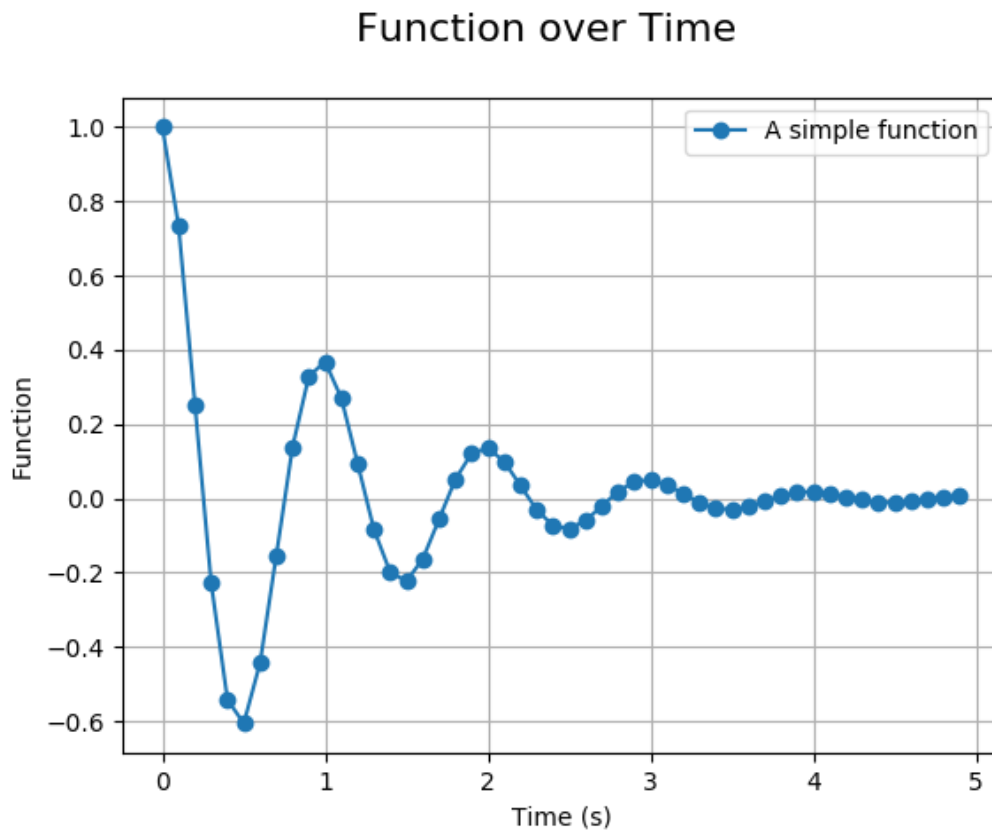
In [4]:

```
# Only for jupyter  
%matplotlib notebook  
  
# import can be done at any time,  
# but best practice tells us to put all of them at the top of the file  
import matplotlib.pyplot as plt  
  
# The simplest plot  
plt.figure()  
plt.plot(t, f(t))  
plt.show()
```



In [5]:

```
# A better plot
fig= plt.figure()
ax = plt.subplot(111)
plt.plot(t, f(t), "-o", label=f.__doc__) # we can access the docstring of f
ax.set_xlabel("Time (s)")
ax.set_ylabel("Function")
plt.suptitle("Function over Time", fontsize=16)
plt.legend()
ax.grid('on')
plt.show()
```



Some interactivity is possible (not easy)

In [5]:

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

def f(t, alpha):
    """
    A simple function with a parameter
    """
    return np.exp(-t) * np.cos(alpha * 2 * np.pi * t)

# Some time steps
nt = 500
t = np.linspace(0.0, 5.0, nt)

# Some parameters
na = 5
alpha = np.logspace(0., 1., na)

# Produce data
data = np.empty((na,2,nt))
for i, a in enumerate(alpha):
    data[i] = t, f(t, a)

# Produce markers
markers = data[:, :, ::10]
```

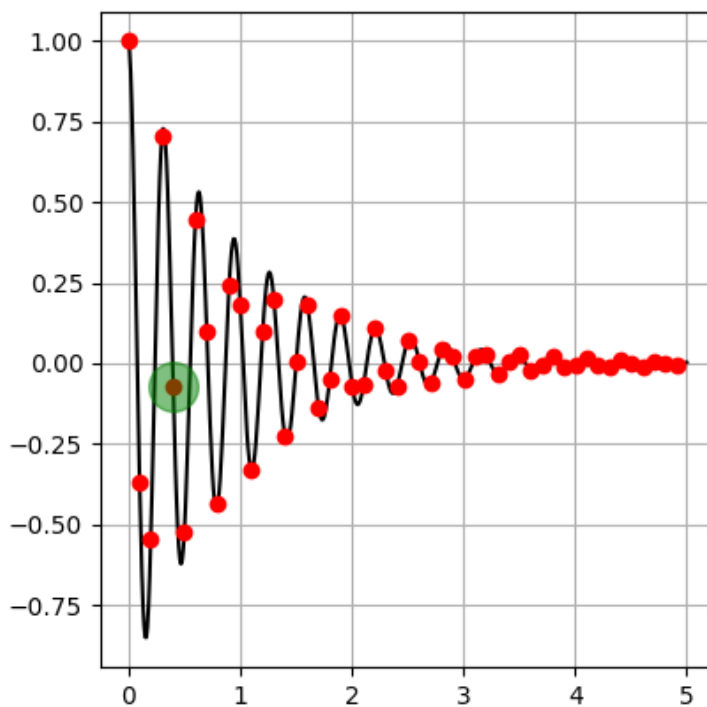
In [6]:

```
from Picker import Picker # An home-made module

def dataplot(ax, ImgNum, args):
    """
    A function that plot the data and the pickable markers
    and return the plot of the pickable markers
    The signature of this function is non-negotiable (forced by Picker)
    """
    data, markers = args
    ax.plot(*data[ImgNum], '-k')
    ax.grid('on')
    plot, = ax.plot(*markers[ImgNum], 'ro', picker=50.)
    return plot

#For jupyter, keep this object in memory
picker = Picker()

# let the user pick one point per image (the first dim of data)
result = picker.pick((data, markers), ndata=na, plotfx=dataplot)
```



Id	X	Y
0	1.00	0.37
1		
2	0.40	-0.07
3		
4		

Previous

Next

In [7]:

```
print(result)

[[ 1.00200401  0.36711384]
 [          nan          nan]
 [ 0.4008016  -0.0732721 ]
 [          nan          nan]
 [          nan          nan]]
```

First exercise : statistics

In [8]:

```
# Load more data
data = np.loadtxt('data/populations.txt').astype(np.int)
print(data)
```

```
[[ 1900 30000  4000 48300]
 [ 1901 47200  6100 48200]
 [ 1902 70200  9800 41500]
 [ 1903 77400 35200 38200]
 [ 1904 36300 59400 40600]
 [ 1905 20600 41700 39800]
 [ 1906 18100 19000 38600]
 [ 1907 21400 13000 42300]
 [ 1908 22000  8300 44500]
 [ 1909 25400  9100 42100]
 [ 1910 27100  7400 46000]
 [ 1911 40300  8000 46800]
 [ 1912 57000 12300 43800]
 [ 1913 76600 19500 40900]
 [ 1914 52300 45700 39400]
 [ 1915 19500 51100 39000]
 [ 1916 11200 29700 36700]
 [ 1917  7600 15800 41800]
 [ 1918 14600  9700 43300]
 [ 1919 16200 10100 41300]
 [ 1920 24700  8600 47300]]
```

In [9]:

```
import numpy as np

# Extract each collumn into a specific vector

# Copy the data array without the year collumn

# Compute for each species
# - the mean population
# - the standard deviation
# - The year when this species had it's maximum of population
# - The two years when this species had it's minimum of population

# Print all that in an table
```

Solution

In [10]:

```
import numpy as np

# Extract each column into a specific vector
years, hares, lynxes, carrots = data.T # unpacking

# Copy the data array without the year column
populations = data[:,1:] # slicing

# Compute for each species
# - the mean population
means = populations.mean(axis=0)

# - the standard deviation
stds = populations.std(axis=0)

# - The year when this species had it's maximum of population
max_populations = np.argmax(populations, axis=0) # use of axis
max_years = years[max_populations] # slicing with a vector
h = a vector

# - The two years when this species had it's minimum of population
lowest_2_pop = np.argsort(populations, axis=0)[:2]
lowest_2_year = years[lowest_2_pop] # slicing with a matrix

# Print all that in an table

format_title = "{:<30} {:^10} | {:^10} | {:^10}"
format_array = "{:<30} {:^10.3e} | {:^10.3e} | {:^10.3e}"
print(format_title.format("", "Hares", "Lynxes", "Carrots"))
print(format_array.format("Mean:", *means)) # unpacking
(rare)
print(format_array.format("Std:", *stds))
print(format_array.format("Max. year:", *max_years))
print(format_array.format("lowest populations year 1:", *lowest_2_year[0]))
print(format_array.format("lowest populations year 2:", *lowest_2_year[1]))
```

	Hares	Lynxes	Carrots
Mean:	3.408e+04	2.017e+04	4.240e+04
Std:	2.090e+04	1.625e+04	3.323e+03
Max. year:	1.903e+03	1.904e+03	1.900e+03
lowest populations year 1:	1.917e+03	1.900e+03	1.916e+03
lowest populations year 2:	1.916e+03	1.901e+03	1.903e+03

In [11]:

```
# All years when at least one specie was above 50000
```

Solution

In [12]:

```
above_50000 = np.any(populations > 50000, axis=1)
print("Any above 50000:", years[above_50000])           # slicing with a mask
```

Any above 50000: [1902 1903 1904 1912 1913 1914 1915]

In [13]:

```
# Dominants species throught the years
```

Solution

In [14]:

```
max_species = np.argmax(populations, axis=1)
species = np.array(['Hare', 'Lynx', 'Carrot'])

max_species=np.stack((years,species[max_species]), axis=1)
print("Max species:")
print(max_species)
```

Max species:

```
[['1900' 'Carrot']
 ['1901' 'Carrot']
 ['1902' 'Hare']
 ['1903' 'Hare']
 ['1904' 'Lynx']
 ['1905' 'Lynx']
 ['1906' 'Carrot']
 ['1907' 'Carrot']
 ['1908' 'Carrot']
 ['1909' 'Carrot']
 ['1910' 'Carrot']
 ['1911' 'Carrot']
 ['1912' 'Hare']
 ['1913' 'Hare']
 ['1914' 'Hare']
 ['1915' 'Lynx']
 ['1916' 'Carrot']
 ['1917' 'Carrot']
 ['1918' 'Carrot']
 ['1919' 'Carrot']
 ['1920' 'Carrot']]
```

In [15]:

```
# Compute the correlation coeficient between the variation of hares and lynxes
```

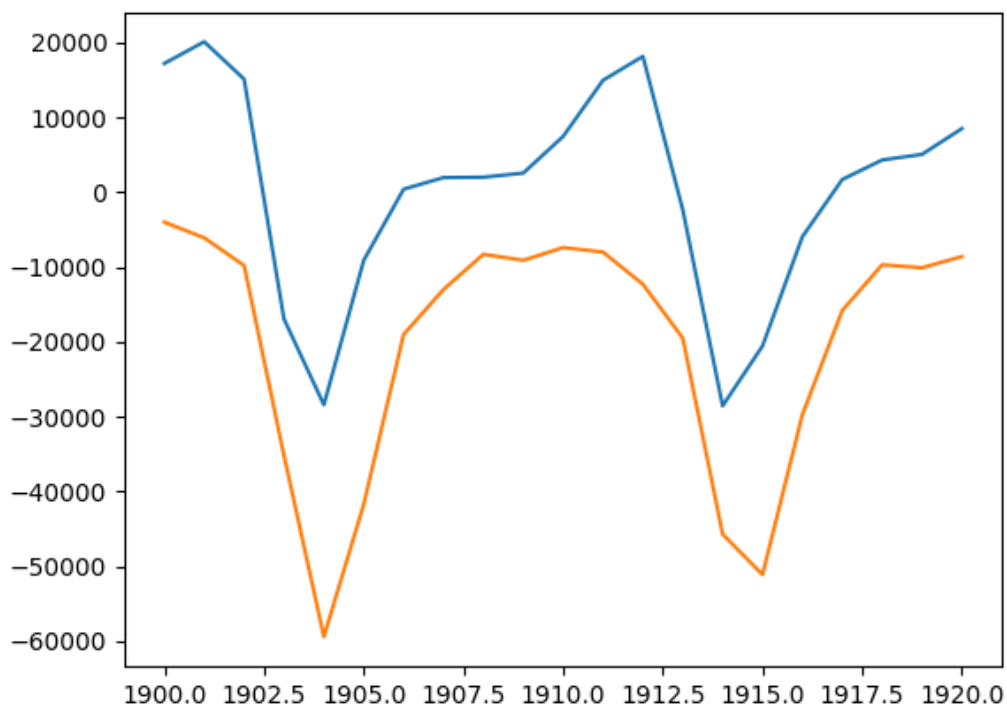
Solution

In [16]:

```
hare_grad = np.gradient(hares, 1.0)

plt.figure()
plt.plot(years, hare_grad)
plt.plot(years, -lynxes)
plt.show()

# Compute the correlation coefficient between the variation of hares and lynxes
print("diff(Hares) vs. Lynxes correlation = ", np.corrcoef(hare_grad, -lynxes)[0
, 1])
```



diff(Hares) vs. Lynxes correlation = 0.9179248480315341

Alternative : Panda

- Excel-like processing

In [17]:

```
import pandas as pd
import numpy as np
# Load data
data = pd.read_csv('data/populations.txt', sep="\t", dtype=np.int, index_col=0)
# fix the year title
data.index.names = ['year']
data.style
```

Out[17]:

	hare	lynx	carrot
year			
1900	30000	4000	48300
1901	47200	6100	48200
1902	70200	9800	41500
1903	77400	35200	38200
1904	36300	59400	40600
1905	20600	41700	39800
1906	18100	19000	38600
1907	21400	13000	42300
1908	22000	8300	44500
1909	25400	9100	42100
1910	27100	7400	46000
1911	40300	8000	46800
1912	57000	12300	43800
1913	76600	19500	40900
1914	52300	45700	39400
1915	19500	51100	39000
1916	11200	29700	36700
1917	7600	15800	41800
1918	14600	9700	43300
1919	16200	10100	41300
1920	24700	8600	47300

In [18]:

```
data.describe().style.format("{:.0f}")
```

Out[18]:

	hare	lynx	carrot
count	21	21	21
mean	34081	20167	42400
std	21414	16656	3405
min	7600	4000	36700
25%	19500	8600	39800
50%	25400	12300	41800
75%	47200	29700	44500
max	77400	59400	48300

In [19]:

```
# Compute for each species
# - the mean population
means = data.mean()
means.name = "Mean"

# - the standard deviation
stds = data.std()
stds.name = "Std"

# - The year when this species had it's maximum of population
max_populations = data.idxmax()
max_populations.name = "Max. year"

# - The two years when this species had it's minimum of population
lowest_2_pop = data.values.argsort(axis=0)[:2]
lowest_2_year = data.index[lowest_2_pop].values

lowest_2_year = pd.DataFrame(lowest_2_year,
                             columns=data.columns,
                             index=["Lowest populations year 1", "Lowest populations year 2"])

# Print all that in an table
result_table = pd.concat([means, stds, max_populations, lowest_2_year.T], axis=1)
result_table.style
```

Out[19]:

	hare	lynx	carrot
Mean	34081	20166.7	42400
Std	21414	16656	3404.56
Max. year	1903	1904	1900
Lowest populations year 1	1917	1900	1916
Lowest populations year 2	1916	1901	1903

In [20]:

```
# All years when at least one specie was above 50000
above_50000 = (data > 50000).any(axis=1)
print("Any above 50000:", data.index[above_50000].values)

# Dominants species throught the years

print("Max species:")
print(data.idxmax(axis=1))
```

Any above 50000: [1902 1903 1904 1912 1913 1914 1915]

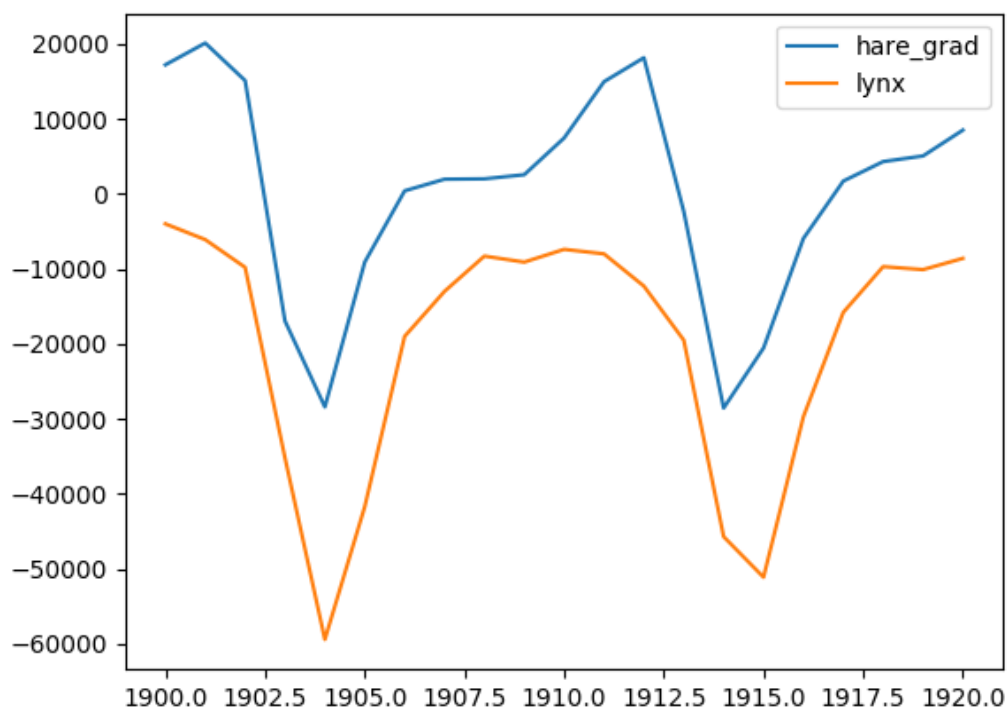
Max species:

```
year
1900    carrot
1901    carrot
1902      hare
1903      hare
1904     lynx
1905     lynx
1906    carrot
1907    carrot
1908    carrot
1909    carrot
1910    carrot
1911    carrot
1912      hare
1913      hare
1914      hare
1915     lynx
1916    carrot
1917    carrot
1918    carrot
1919    carrot
1920    carrot
dtype: object
```


In [21]:

```
data["hare_grad"] = np.gradient(data["hare"], data.index.to_series())

plt.figure()
plt.plot(data["hare_grad"])
plt.plot(-data["lynx"])
plt.legend()
plt.show()
```



In [22]:

```
# Compute the correlation coefficient between the variation of hares and lynxes
print("Correlation")
print(data.corr())
```

Correlation

	hare	lynx	carrot	hare_grad
hare	1.000000	0.071892	-0.016604	-0.006390
lynx	0.071892	1.000000	-0.680577	-0.917925
carrot	-0.016604	-0.680577	1.000000	0.718199
hare_grad	-0.006390	-0.917925	0.718199	1.000000

Image processing

pillow

For reading and writing images in a lot of format (tif, jpeg, ...)

Opencv

For image processing but usually scikit-image is better (but opencv is more complete)

scikits

'Plugins' for scipy <http://scikits.appspot.com/scikits> (<http://scikits.appspot.com/scikits>) e.g. scikit-image

Exemple

In [22]:

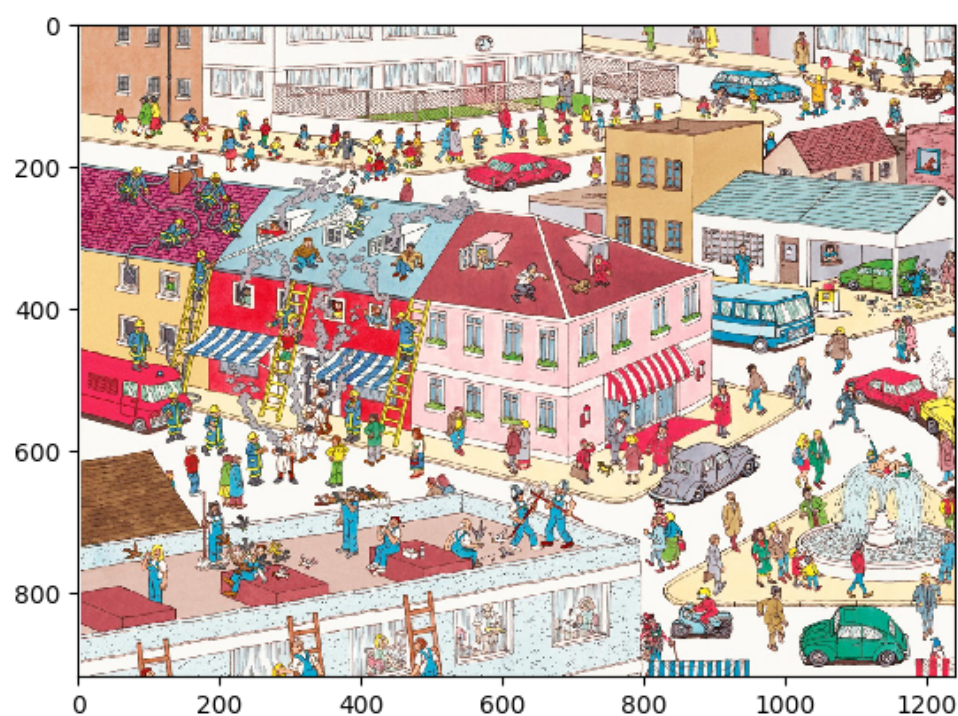
```
%matplotlib notebook
```

```
from PIL import Image  
waldo = Image.open("data/waldo.jpg")  
waldo = np.array(waldo)
```

```
print(waldo.shape, waldo.dtype)
```

```
plt.figure()  
plt.imshow(waldo)  
plt.show()
```

```
(917, 1240, 3) uint8
```



In [23]:

```
%matplotlib notebook

# Make a copy of the image
solution = waldo.copy()

# An image is a 2d Array (3d with for colored image)
# I need indices of pixels (x and y)
sy, sx, sc = waldo.shape
y, x, c = np.mgrid[0:sy, 0:sx, 0:sc]
# Approximate position of waldo
centerx, centery = (810, 870)
size = 50

# Darken everything except a circle around the waldo
mask = ((y - centery) ** 2 + (x - centerx) ** 2) > size ** 2
solution[mask] /= 2

# Plot the solution
plt.figure()
plt.imshow(solution)
plt.show()
```



Exercise

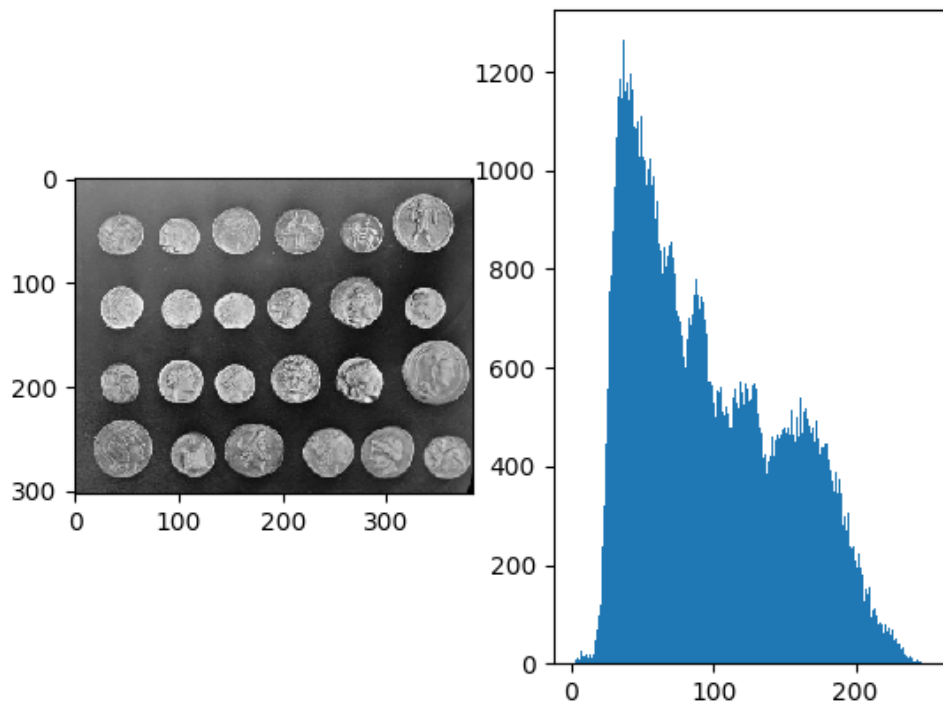
We have an image of some coins on a dark background.
We want to extract those coins

In [24]:

```
%matplotlib notebook
from scipy import ndimage as ndi
from skimage import data
from skimage.color import label2rgb

# get data
coins = data.coins()

# Two plot side by side
# plot coins on the left one
fig, axes = plt.subplots(1,2)
axes[0].imshow(coins, cmap='gray')
# plot the histogram on the right
axes[1].hist(coins.flatten(), bins=np.arange(0, 256))
plt.show()
```



In [25]:

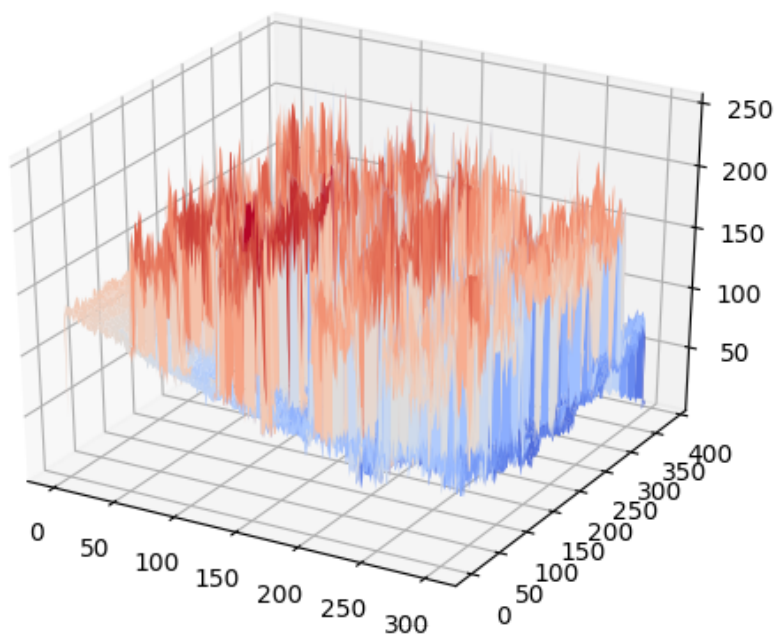
```
# 3D plot

from mpl_toolkits.mplot3d import Axes3D
from matplotlib import cm

sx,sy = coins.shape
x, y = np.mgrid[0:sx, 0:sy]

fig = plt.figure()
ax = fig.add_subplot(111, projection='3d')

ax.plot_surface(x, y, coins, cmap=cm.coolwarm)
plt.show()
```



In [26]:

```
def plot_result(segmentation, title=""):
    # Select a different color for each coin
    labeled_coins, _ = ndi.label(segmentation)
    image_label_overlay = label2rgb(labeled_coins, image=coins)

    fig = plt.figure()
    # The coins
    plt.imshow(coins, cmap=plt.cm.gray)
    # The edge of the segmentation
    plt.contour(segmentation, [0.5], linewidths=1.2, colors='y')
    # Each detected coin in a different color
    plt.imshow(image_label_overlay)

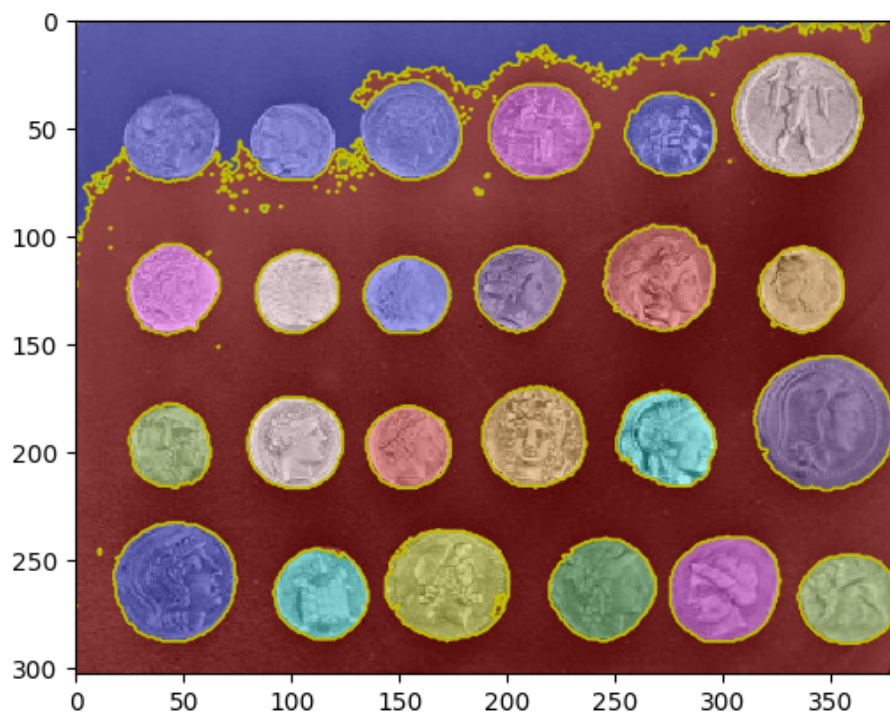
    if title:
        plt.suptitle(title, fontsize=16)
    plt.show()

def segmentation_with_threshold(datain, threshold):
    """ simple segmentation based on a threshold """
    coins = datain > threshold
    # binary_fill_holes is used to remove holes in the coins
    return ndi.binary_fill_holes(coins)
```

In [27]:

```
segmentation_thre = segmentation_with_threshold(coins, 100)
plot_result(segmentation_thre, "Threshold method with {}".format(100))
```

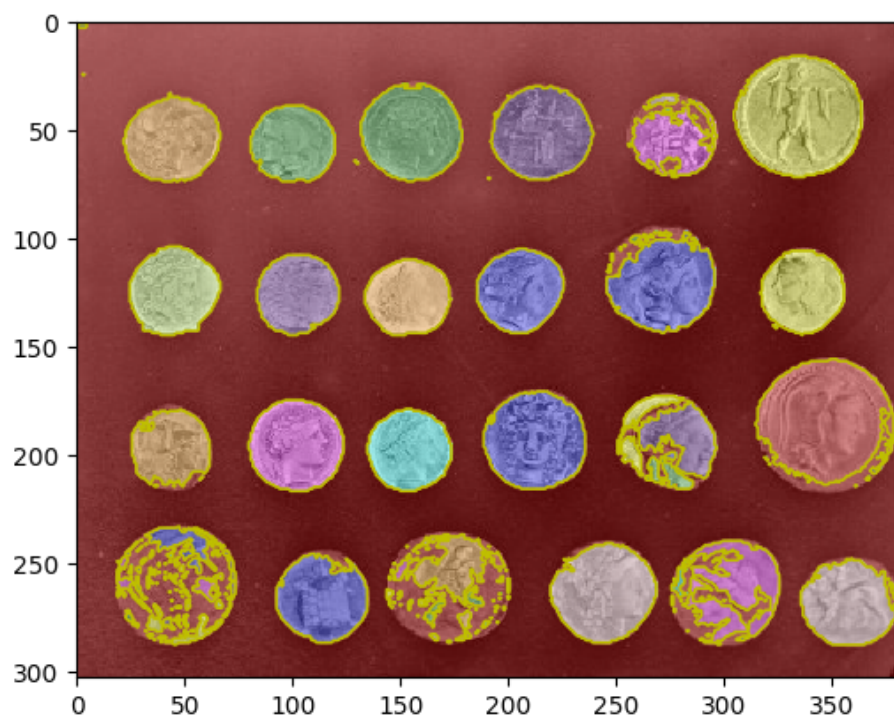
Threshold method with 100



In [28]:

```
segmentation_thre = segmentation_with_threshold(coins, 140)  
plot_result(segmentation_thre, "Threshold method with {}".format(140))
```

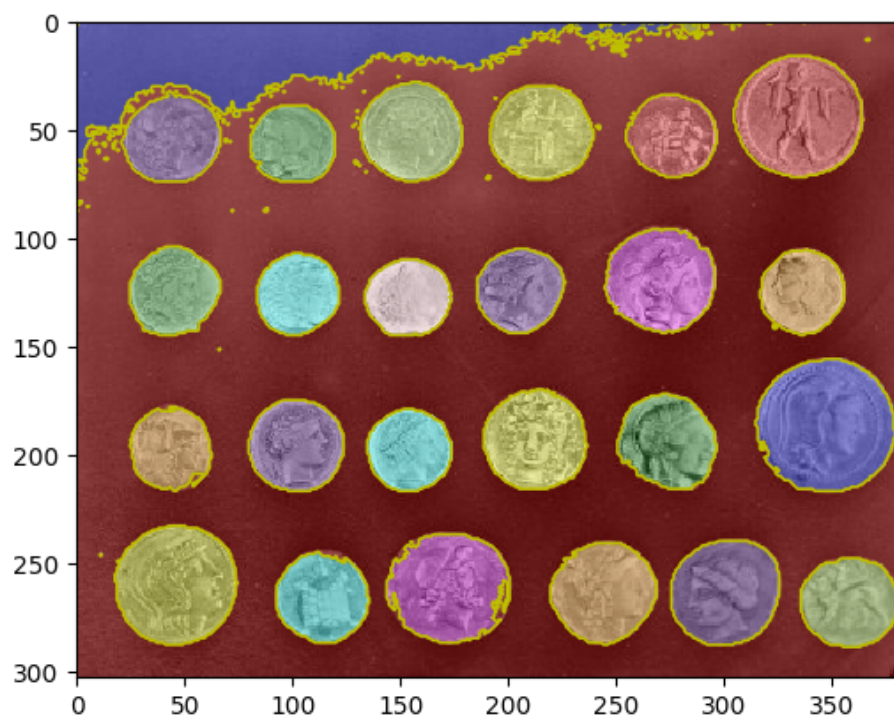
Threshold method with 140



In [29]:

```
segmentation_thre = segmentation_with_threshold(coins, 110)  
plot_result(segmentation_thre, "Threshold method with {}".format(110))
```

Threshold method with 110



In [30]:

```
%matplotlib notebook

from skimage.feature import canny

def segmentation_with_edges(datain):
    """
    Segmentation based on edges
    1 - Apply canny edge filter
    2 - binary_fill_holes
    """
    dataout = datain > 110 # TODO replace this line
    return dataout
```

Solution

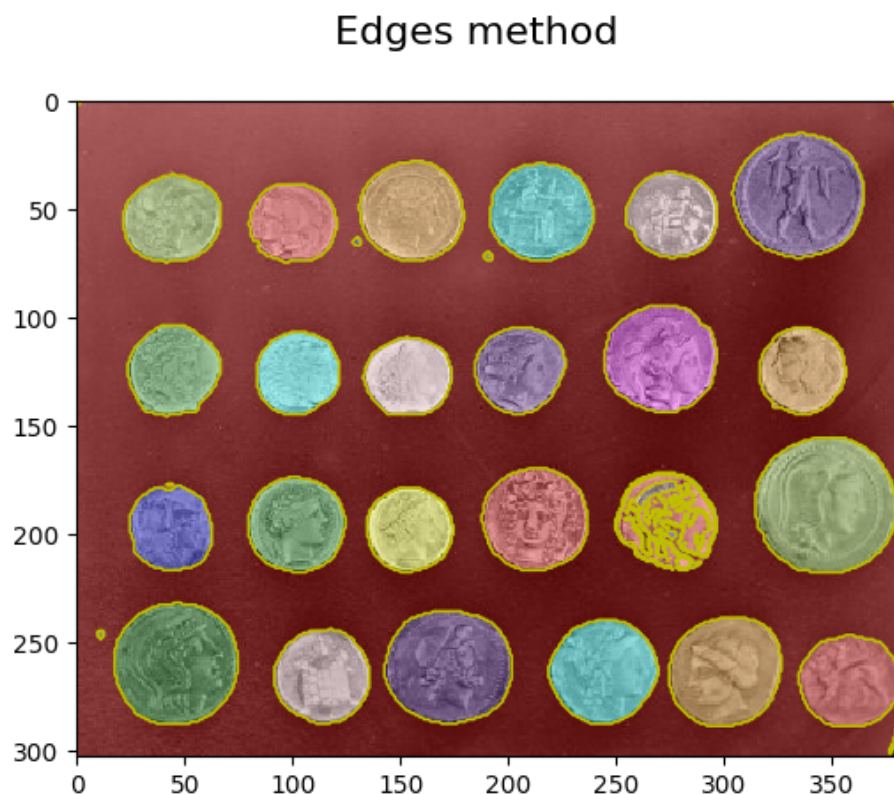
In [31]:

```
from skimage.feature import canny

def segmentation_with_edges(datain):
    """
    Segmentation based on edges
    1 - Apply canny edge filter
    2 - binary_fill_holes
    """
    return ndi.binary_fill_holes(canny(datain))
```

In [32]:

```
segmentation_edges = segmentation_with_edges(coins)
plot_result(segmentation_edges, "Edges method")
```



In [33]:

```
%matplotlib notebook

from skimage.filters import sobel
from skimage.morphology import watershed

def segmentation_with_region(datain):
    """
    Segmentation based on region
    1 - use sobel to compute an elevation map
    2 - mark pixels
        1 for background for sure
        2 for coins for sure
        0 for we don't know
    3 - apply watershed
    4 - binary_fill_holes
    """
    dataout = datain > 110 # TODO replace this line
    return dataout
```

Solution

In [34]:

```
from skimage.filters import sobel
from skimage.morphology import watershed

def segmentation_with_region(datain):
    """
    Segmentation based on region
    1 - use sobel to compute an elevation map
    2 - mark pixels
        1 for background for sure
        2 for coins for sure
        0 for we don't know
    3 - apply watershed
    4 - binary_fill_holes
    """

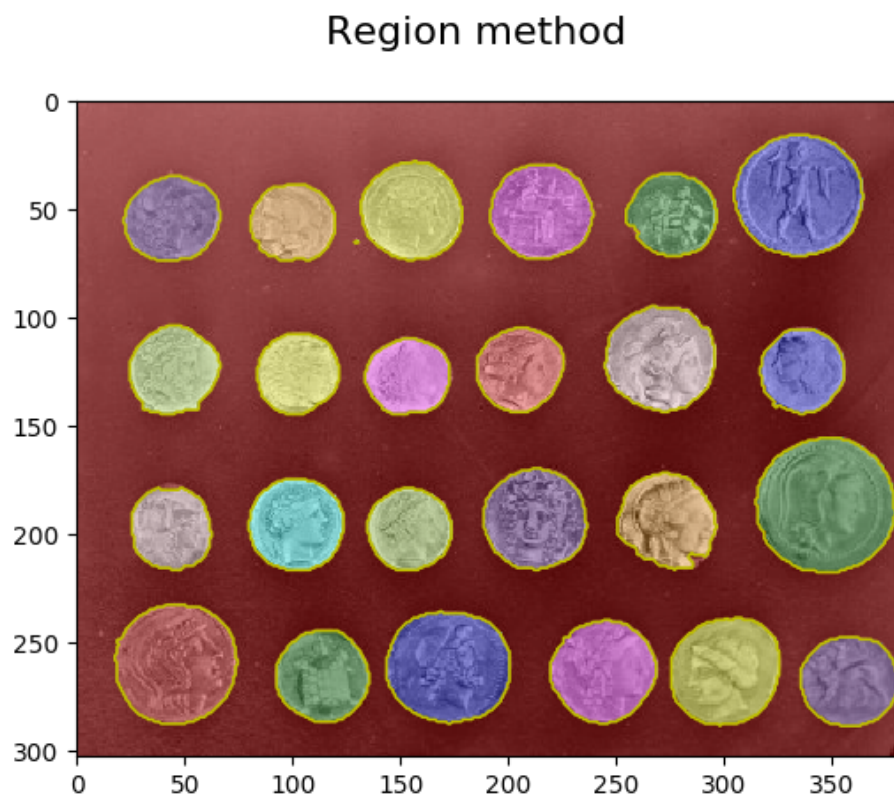
    # use sobel in order to compute elevation map
    elevation_map = sobel(datain)

    # mark pixels
    # 1 for background for sure
    # 2 for coins for sure
    # 0 for we don't know
    markers = np.zeros_like(datain)
    markers[datain < 30] = 1
    markers[datain > 150] = 2

    # apply watershed algo
    segmentation = watershed(elevation_map, markers) - 1
    return ndi.binary_fill_holes(segmentation)
```

In [35]:

```
segmentation_region = segmentation_with_region(coins)  
plot_result(segmentation_region, "Region method")
```



In [36]:

```
%matplotlib notebook

def filter_small_objects(datain, threshold, biggest=False):
    """
    Segmentation based on edges
    1 - use label to labelize each zone
    2 - use bincount to count the number of pixel of each zone
    3 - select which zone to keep after filter
        - based on threshold
        - except background
        - eventually except biggest
    4 - apply filter
    """
    dataout = datain # TODO replace this line
    return dataout
```

Solution

In [37]:

```
def filter_small_objects(datain, threshold, biggest=False):
    """
    Segmentation based on edges
    1 - use label to labelize each zone
    2 - use bincount to count the number of pixel of each zone
    3 - select which zone to keep after filter
        - based on threshold
        - except background
        - eventually except biggest
    4 - apply filter
    """
    # label each zone
    label_objects, nb_labels = ndi.label(datain)
    # size of each zone in pixel
    sizes = np.bincount(label_objects.flatten())
    # Only keep all zone bigger than threshold
    mask_sizes = sizes > threshold

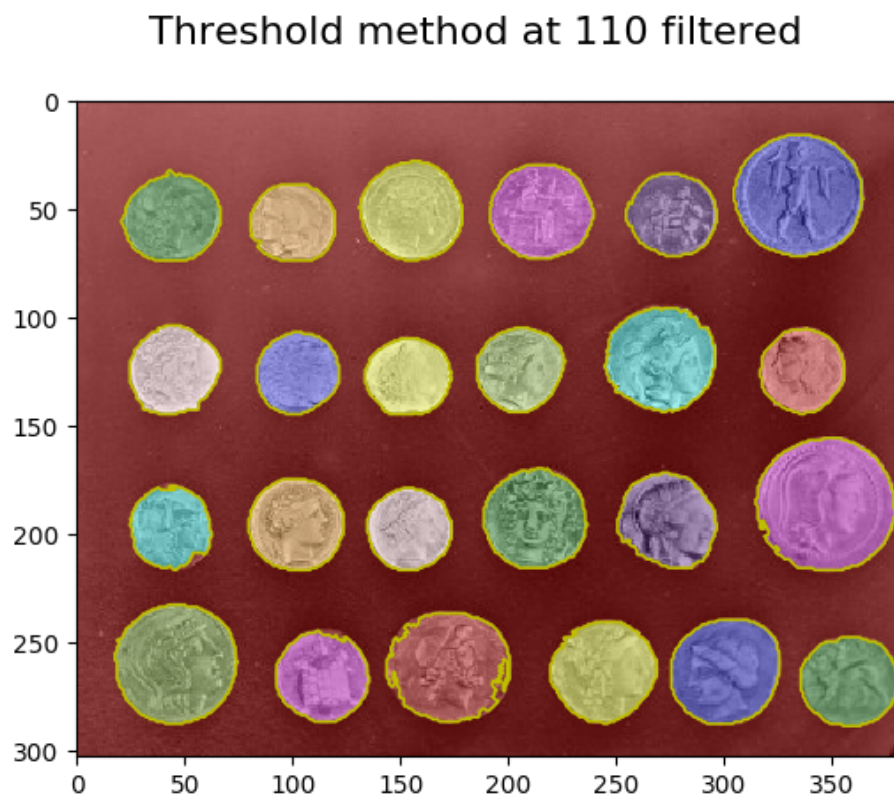
    # remove the background
    mask_sizes[0] = False

    if biggest:
        # remove the biggest zone (except background)
        mask_sizes[np.argsort(sizes)[-2]] = False

    #apply filter
    return mask_sizes[label_objects]
```

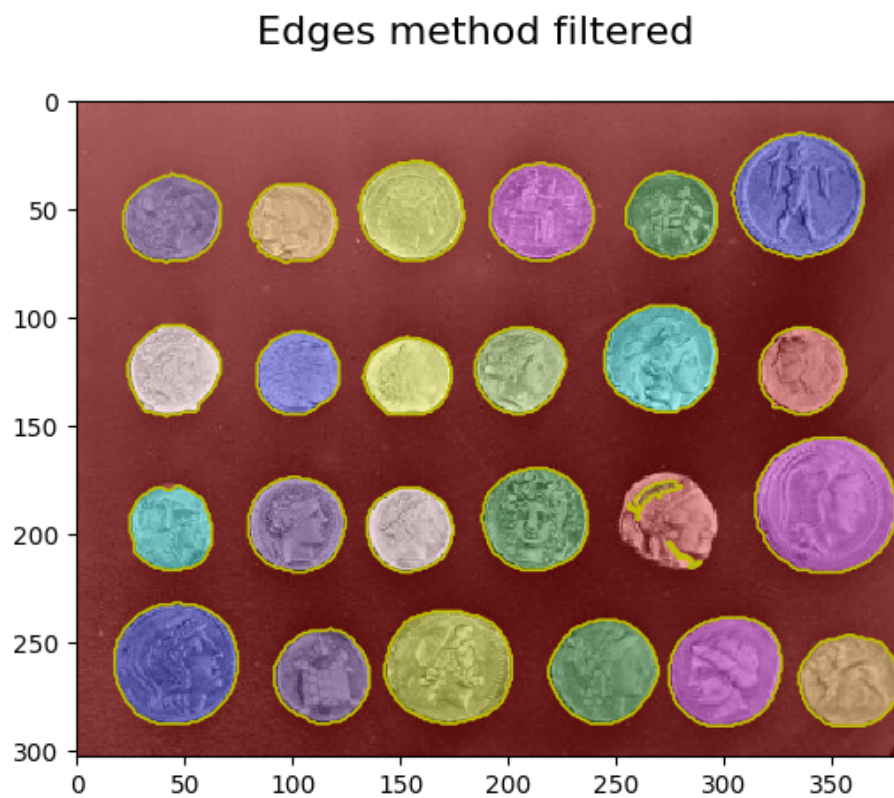
In [38]:

```
segmentation_thre_filt = filter_small_objects(segmentation_thre,50, biggest=True)  
plot_result(segmentation_thre_filt, "Threshold method at 110 filtered")
```



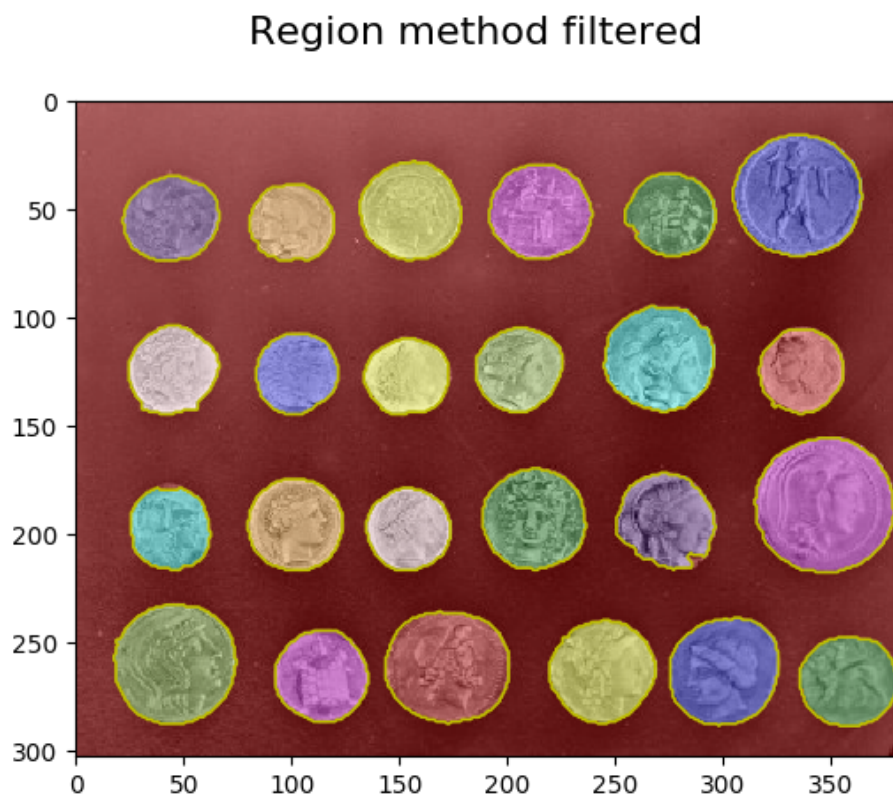
In [39]:

```
segmentation_edges_filt = filter_small_objects(segmentation_edges, 20)  
plot_result(segmentation_edges_filt, "Edges method filtered")
```



In [40]:

```
segmentation_region_filt = filter_small_objects(segmentation_region, 20)
plot_result(segmentation_region_filt, "Region method filtered")
```



In [41]:

```
def filled(datain):
    """
    Try harder to fill holes
    1 - dilation
    2 - binary_fill_holes
    3 - 2*erosion
    4 - dilation
    """
    dataout = datain # TODO replace this line
    return dataout
```

Solution

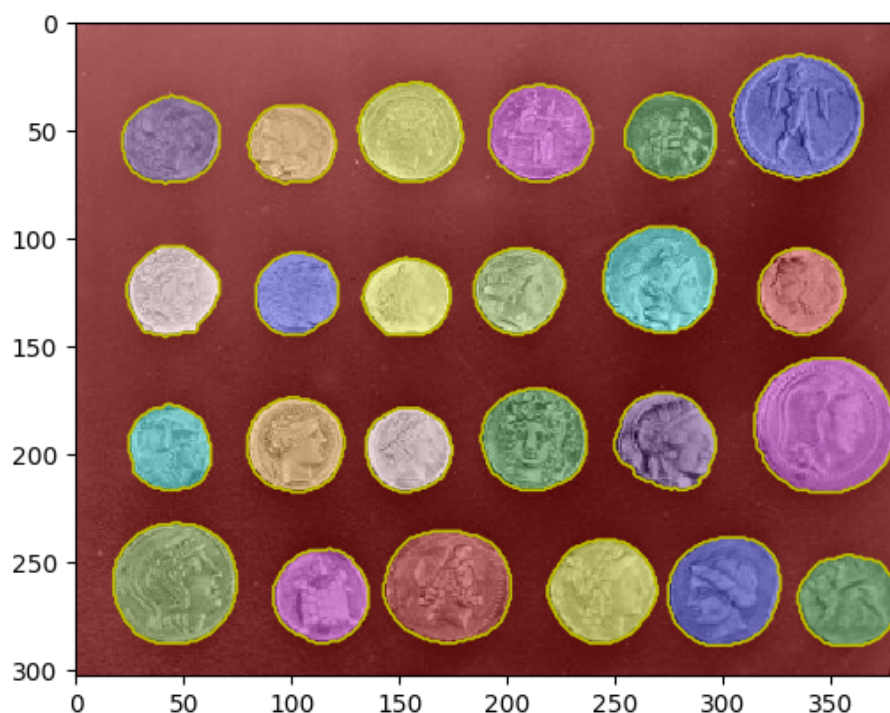
In [42]:

```
def filled(datain):  
    """  
    Try harder to fill holes  
    1 - dilation  
    2 - binary_fill_holes  
    3 - 2*erosion  
    4 - dilation  
    """  
    segmentation_dil = ndi.morphology.binary_dilation(datain, iterations=1)  
    segmentation_filled = ndi.binary_fill_holes(segmentation_dil)  
    segmentation_ero = ndi.morphology.binary_erosion(segmentation_filled, iterations=2)  
    segmentation_final = ndi.morphology.binary_dilation(segmentation_ero, iterations=1)  
    return segmentation_final
```

In [44]:

```
segmentation_edges_fill = filled(segmentation_edges)  
segmentation_edges_fill_filt = filter_small_objects(segmentation_edges_fill, 20)  
plot_result(segmentation_edges_fill_filt, "Edges method filled and filtered")
```

Edges method filled and filtered



Signal processing

Exercise

We have a signal, and we want to do a Lorentz fit on all the peaks

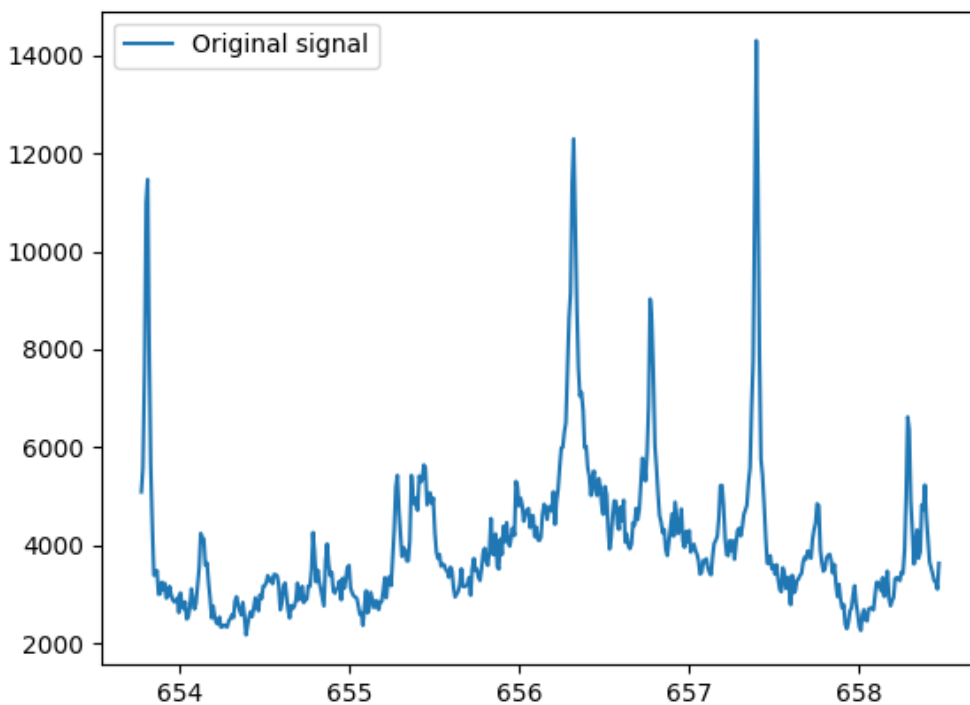
1. filter the signal
2. find peaks on the filtered signal
3. determine window of interest for the fitting
4. apply fit

In [45]:

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

# get data
wavelength, signal = np.loadtxt("data/Tungsten spectrum.dat").T

fig = plt.figure()
plt.plot(wavelength, signal, label="Original signal")
plt.legend()
plt.show()
```



In [46]:

```
from scipy.signal import wiener

def filter(wavelength, signal):
    """
    Filter the signal in order to ease extraction of maxima

    scipy.signal.wiener is a first step
    """

    filtered_signal = signal # TODO #
    return filtered_signal
```

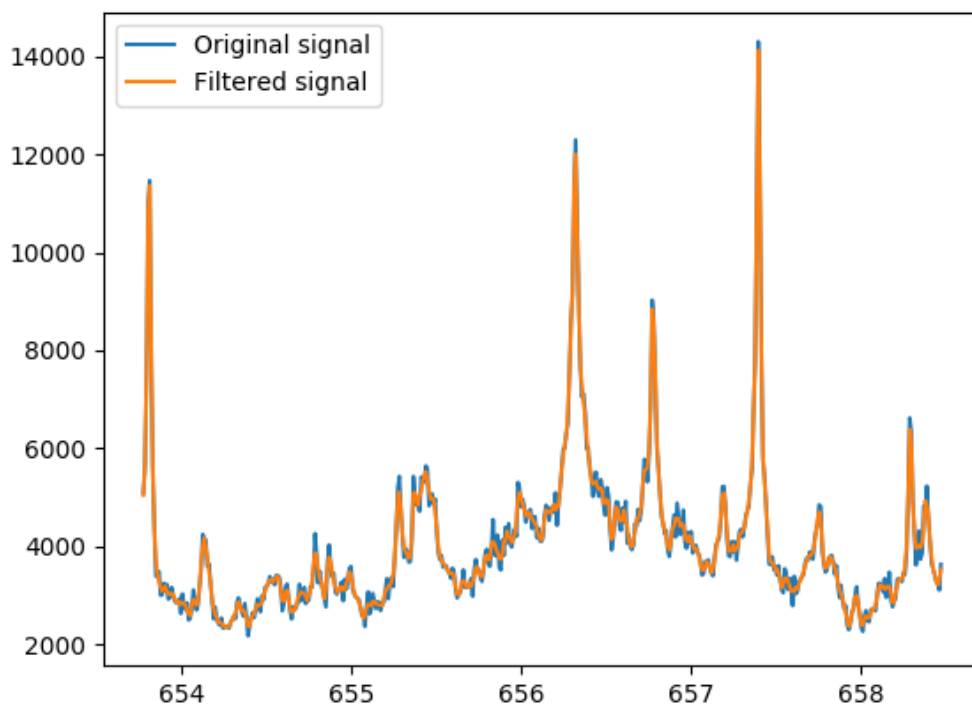
Solution filter

In [47]:

In [48]:

```
filtered_signal = filter(wavelength, signal)

fig = plt.figure()
plt.plot(wavelength, signal, label="Original signal")
plt.plot(wavelength, filtered_signal, label="Filtered signal")
plt.legend()
plt.show()
```



In [49]:

```
from scipy.signal import argrelmax

def find_peaks(wavelength, signal):
    """
    Find some maxima of the signal

    Finding the maximum of the signal is also a first step
    scipy.signal.argrelmax is also a good idea

    indexes_max must be a list (eventually containing only one element)
    """
    indexes_max = [256] # TODO #
    return indexes_max
```

Solution find_peaks

In [50]:

```
from scipy.signal import argrelmax

def find_peaks(wavelength, signal):
    """
    Find some maxima of the signal

    Finding the maximum of the signal is also a first step
    scipy.signal.argrelmax is also a good idea

    indexes_max must be a list (eventually containing only one element)
    """

    indexes_max = argrelmax(signal)[0]
    return indexes_max
```

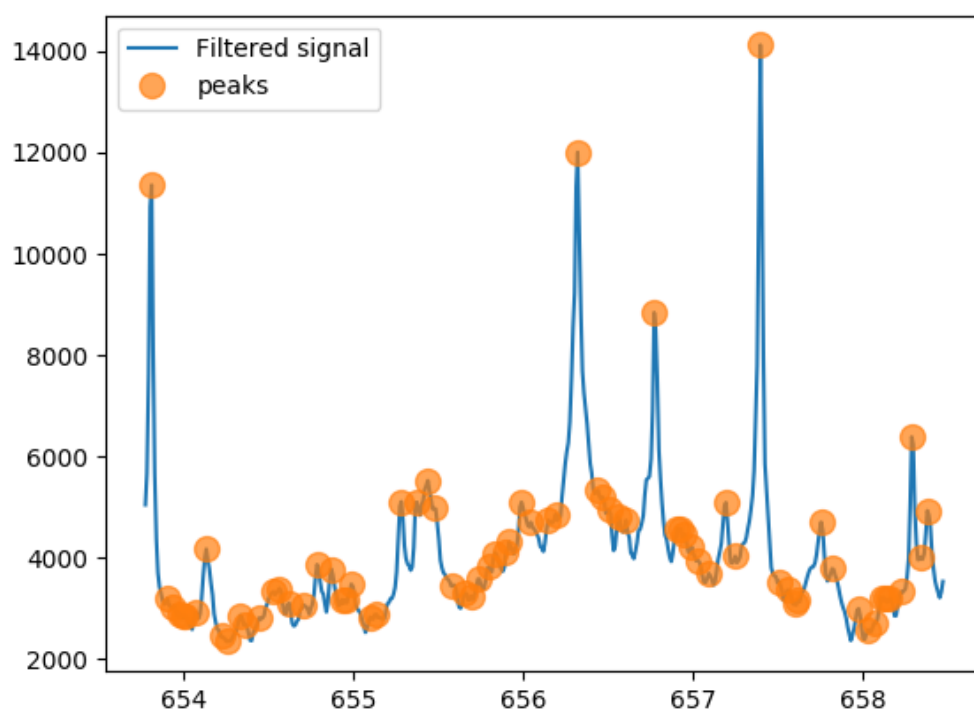
In [51]:

```
maximas = find_peaks(wavelength, filtered_signal)

fig = plt.figure()
plt.plot(wavelength, filtered_signal, label="Filtered signal")

# add a circle on all the peaks
plt.plot(wavelength[maximas], filtered_signal[maximas],
         'o', ms=10, alpha=0.7, label="peaks")

plt.legend()
plt.show()
```



In [52]:

```
from scipy.signal import argrelmin, argrelmax

def get_windows(wavelength, signal, indexes_max):
    """
    Find out window of interest around peaks

    The window of interest is the time range between two local minima around the
    peak

    In order to find it:
    - use scipy.signal.argrelmin to extract all local minimas
    - in a loop for all peak:
      - use numpy.argmax to find the next local minima after the current peak
      - compute the edges of the window, beware of the boundaries
    """

    windows = {}
    for peak in indexes_max:
        windows[peak] = [200, 300] # TODO #

    return windows
```

Solution get_windows

In [53]:

```
from scipy.signal import argrelmin, argrelmax

def get_windows(wavelength, signal, indexes_max):
    """
    Find out window of interest around peaks

    The window of interest is the time range between two local minima around the
    peak

    In order to find it:
    - use scipy.signal.argrelmin to extract all local minimas
    - in a loop for all peak:
      - use numpy.argmax to find the next local minima after the current peak
      - compute the edges of the window, beware of the boundaries
    """

    windows = {}

    # get index of the minimas
    minimas = argrelmin(signal)[0]

    for peak in indexes_max:

        # get index of the next minima in minimas
        next_minima = np.argmax(minimas > peak)

        # if there is no minima after the peak
        if minimas[next_minima] < peak:
            wmax = len(signal) - 1
        else:
            wmax = minimas[next_minima]

        # if there is no minima before the peak
        if next_minima == 0:
            wmin = 0
        else:
            wmin = minimas[next_minima-1]

        windows[peak] = [wmin, wmax]

    return windows
```


In [54]:

```
def filter_peaks(windows):
    """
    Filter out unusable peaks
    A peak is unusable when the window is too short (less than 5 values)

    Create a new dictionary containing only usable peaks
    """
    filtered_windows = {}
    for peak, (wmin, wmax) in windows.items():
        if wmax - wmin >= 5:
            filtered_windows[peak] = [wmin, wmax]
    return filtered_windows

def get_minmaxpeaks(windows):
    """
    Extract a list of all extrema that we will use
    """
    limits = np.asarray(list(windows.values())).flatten()
    maxpeaks = list(windows.keys())
    return limits, maxpeaks

# Get peaks
windows = get_windows(wavelength, filtered_signal, maximas)
peaks = filter_peaks(windows)

selected_limits, selected_maxpeaks = get_minmaxpeaks(peaks)

# start plot
fig = plt.figure()
ax = plt.subplot(111)

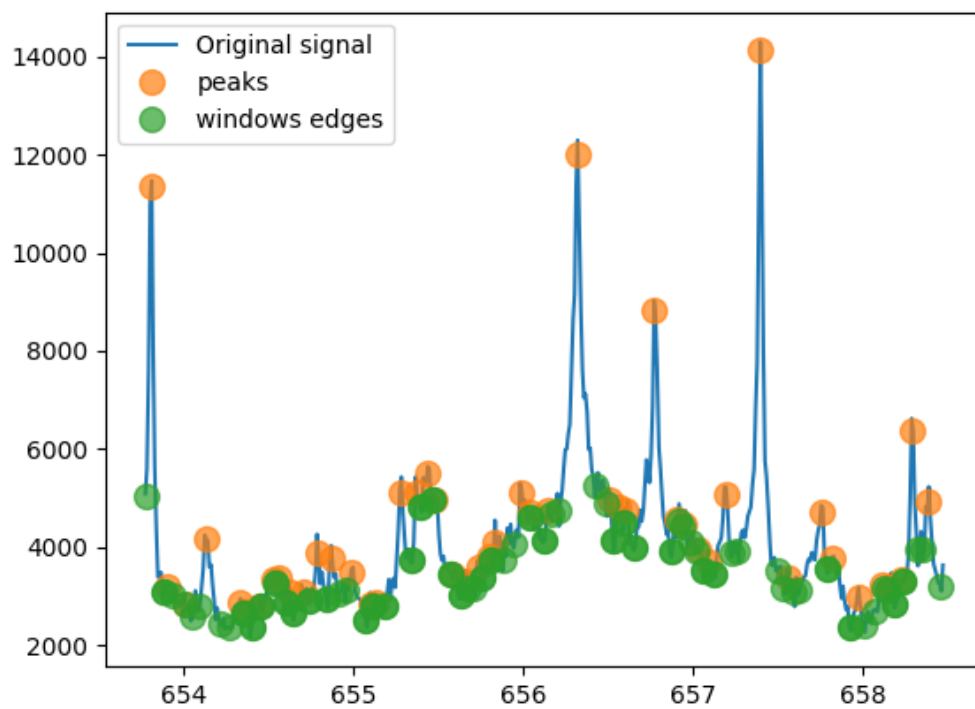
# plot the signal
plt.plot(wavelength, signal, label="Original signal")
# plt.plot(wavelength, filtered_signal, label="Filtered signal")

# add a circle on all the peaks
plt.plot(wavelength[selected_maxpeaks],
         filtered_signal[selected_maxpeaks],
         'o', ms=10, alpha=0.7, label="peaks")

# add a circle on the limit of the windows
plt.plot(wavelength[selected_limits],
         filtered_signal[selected_limits],
         'o', ms=10, alpha=0.7, label="windows edges")

plt.legend()

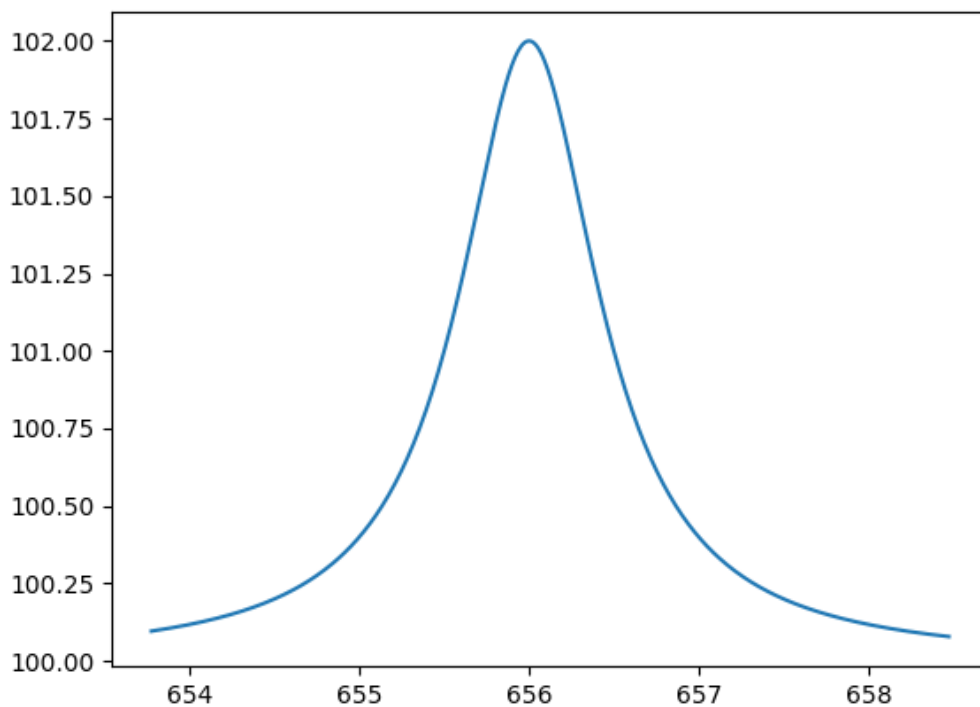
# finish plotting
plt.show()
```



In [55]:

```
%matplotlib notebook
```

```
def lorentz(param, peak, x):  
    """  
    Lorentz function  
    - param is a vector of 3 parameter : baseline, gamma and amplitude  
    The optimisation will adjust them  
  
    - peak is the position of the peak  
    - x is the points of evaluation of the function  
    """  
    baseline, gamma, amplitude = param  
  
    num = 2 / (np.pi * gamma)  
    denom = 1 + ((x - peak) / (gamma / 2)) ** 2  
    fx = num / denom  
  
    maxlorentz = fx.max()  
  
    return baseline + amplitude * fx / maxlorentz  
  
param = (100, 1, 2)  
y = lorentz(param, 656, wavelength)  
  
plt.figure()  
plt.plot(wavelength, y)  
plt.show()
```



In [56]:

```
from scipy.optimize import minimize

def lorentz_fit(wavelength, signal, peak, window):
    """
    Compute a fit of a lorentz function around the peak inside a window
    1 - define a cost function (e.g. least square)
    2 - extract the window of interest
    3 - choose appropriate initial value on the 3 lorentz parameter
    4 - apply the *minimize* procedure to optimize those parameter
        use the *args* argument in order to pass more arguments
    5 - return the optimal parameters and the resulting fit
    """

    def cost(param, peak, x, signal):
        """
        Compute the error between a lorentz fit and a signal
        1 - compute the resulting fit
        2 - compute the error
        """
        fit = lorentz(param, peak, x)
        error = np.sqrt(np.sum((fit - signal) ** 2))
        return error

    # extract data for fitting

    # initial values for baseline, gamma and amplitude
    init_param = [1., 1., 1.]

    # fitting
    opt_param = init_param # TODO #

    fit = lorentz(opt_param, peak, wavelength)

    return opt_param, (wavelength, fit)
```

Solution lorentz_fit

In [57]:

```
from scipy.optimize import minimize

def lorentz_fit(wavelength, signal, peak, window):
    """
    Compute a fit of a lorentz function around the peak inside a window
    1 - define a cost function (e.g. least square)
    2 - extract the window of interest
    3 - choose appropriate initial value on the 3 lorentz parameter
    4 - apply the *minimize* procedure to optimize those parameter
        use the *args* argument in order to pass more arguments
    5 - return the optimal parameters and the resulting fit
    """

    def cost(param, peak, x, signal):
        """
        Compute the error between a lorentz fit and a signal
        1 - compute the resulting fit
        2 - compute the error
        """
        fit = lorentz(param, peak, x)
        error = np.sqrt(np.sum((fit - signal) ** 2))
        return error

    # extract data for fitting
    wmin, wmax = window
    wavelength = wavelength[wmin:wmax]
    signal = signal[wmin:wmax]

    # initial values for baseline, gamma and amplitude
    init_param = [2000., 0.1, 4000]

    # fitting
    res = minimize(cost, init_param, args=(peak, wavelength, signal))
    opt_param = res.x

    fit = lorentz(opt_param, peak, wavelength)

    return opt_param, (wavelength, fit)
```

In [58]:

```
# start plot
fig= plt.figure()
ax = plt.subplot(111)

# plot the signal
plt.plot(wavelength, signal, label="Original signal")
#plt.plot(wavelength, filtered_signal, label="Filtered signal")

# add a circle on all the peaks
if False:
    plt.plot(wavelength[selected_maxpeaks],
             filtered_signal[selected_maxpeaks],
             'o', ms=10, alpha=0.7, label="peaks")

# add a circle on the limit of the windows
if False:
    plt.plot(wavelength[selected_limits],
             filtered_signal[selected_limits],
             'o', ms=10, alpha=0.7, label="base for fit")

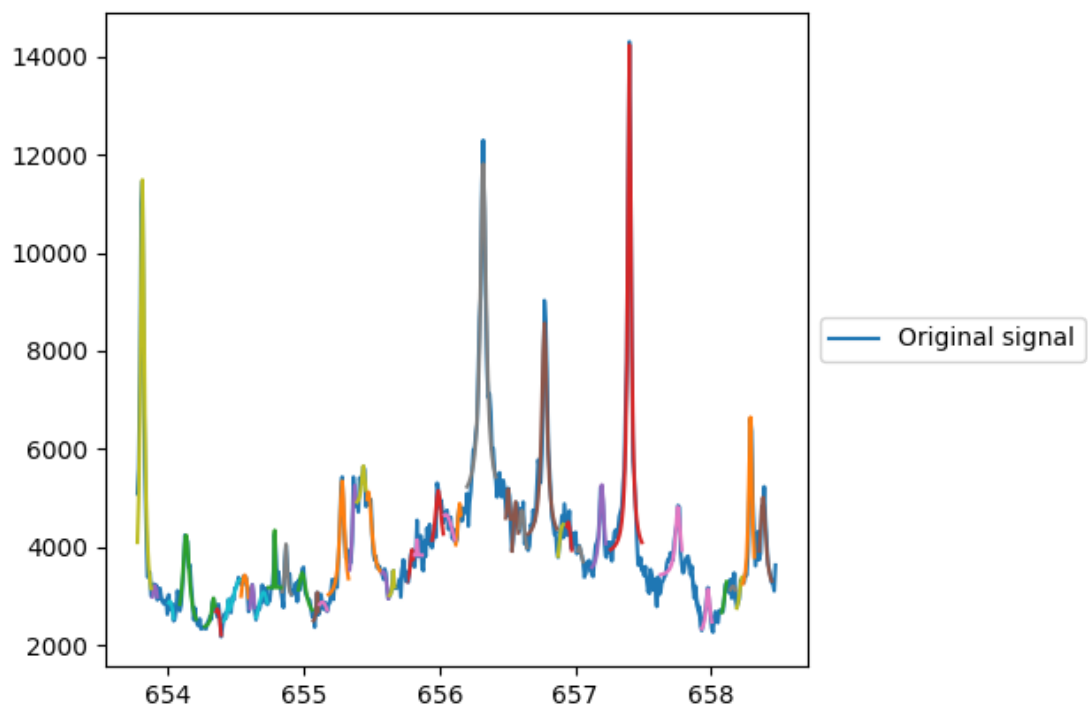
# Apply fit on all peaks
print("{:^8}" + " | {:^9}" * 3).format("Peak", "Baseline", "Gamma", "Amplitude")
)
for key, window in peaks.items():
    peak = wavelength[key]

    param, fit = lorentz_fit(wavelength, signal, peak, window)
    print("{:8.2f}" + " | {:9.2e}" * 3).format(peak, *param))

    # plot
    plt.plot(fit[0], fit[1])

# Put a legend to the right of the current axis
box = ax.get_position()
ax.set_position([box.x0, box.y0, box.width * 0.8, box.height])
ax.legend(loc='center left', bbox_to_anchor=(1, 0.5))

# finish plotting
plt.show()
```



Peak	Baseline	Gamma	Amplitude
656.15	3.68e+03	3.73e-02	1.21e+03
654.99	2.55e+03	6.96e-02	9.31e+02
657.40	3.83e+03	3.00e-02	1.04e+04
653.90	-7.91e+03	2.47e-01	1.11e+04
655.10	2.47e+03	1.33e-02	6.09e+02
655.14	-1.63e+03	3.68e-01	4.51e+03
656.32	4.92e+03	5.16e-02	6.89e+03
653.81	2.59e+03	3.35e-02	8.90e+03
654.01	-8.36e+03	3.13e-01	1.13e+04
657.56	2.98e+03	3.57e-02	4.44e+02
655.28	2.93e+03	4.27e-02	2.41e+03
654.13	2.27e+03	5.84e-02	1.98e+03
655.80	3.18e+03	3.20e-02	7.69e+02
655.38	2.91e+03	4.48e-02	2.35e+03
656.56	2.62e+03	6.16e-02	2.31e+03
657.76	3.40e+03	4.41e-02	1.42e+03
656.61	3.61e+03	5.21e-02	1.14e+03
655.44	4.84e+03	3.09e-02	8.18e+02
654.45	2.46e+03	2.34e-02	4.65e+02
657.82	1.60e+03	1.78e-01	2.14e+03
655.48	3.31e+03	6.05e-02	1.81e+03
654.34	2.35e+03	3.29e-02	6.13e+02
654.36	-1.68e+04	3.35e-01	1.95e+04
655.59	-1.50e+04	4.25e-01	1.85e+04
656.77	4.11e+03	4.62e-02	4.46e+03
657.98	2.23e+03	3.39e-02	9.12e+02
654.87	2.95e+03	2.12e-02	1.11e+03
655.66	2.98e+03	1.41e-02	5.40e+02
654.53	2.08e+03	1.51e-01	1.26e+03
655.73	3.18e+03	2.05e-02	5.60e+02
654.57	-5.65e+03	2.42e-01	9.08e+03
658.12	2.46e+03	4.31e-02	8.41e+02
656.95	3.03e+03	6.78e-02	1.48e+03
654.62	2.28e+03	3.73e-02	9.49e+02
656.51	4.35e+03	2.27e-02	8.28e+02
655.84	3.84e+03	2.52e-04	3.11e+02
657.03	3.51e+03	4.12e-02	4.99e+02
658.23	2.55e+03	4.29e-02	8.34e+02
654.70	2.12e+03	1.02e-01	9.69e+02
657.10	3.06e+03	5.77e-02	6.59e+02
658.29	3.01e+03	2.94e-02	3.64e+03
654.79	3.18e+03	1.58e-04	1.16e+03
655.99	3.78e+03	5.55e-02	1.38e+03
657.20	3.46e+03	4.00e-02	1.81e+03
658.38	3.05e+03	5.01e-02	1.97e+03
656.05	3.05e+03	1.91e-01	1.61e+03
658.16	-1.02e+03	2.73e-01	4.23e+03
656.91	-2.11e+04	4.62e-01	2.56e+04

Exemple : EDO

In [59]:

```
def tank(t, y):
    """
    Dynamic balance for a CSTR

    C_A = y[0] = the concentration of A in the tank, [mol/L]
    T = y[1] = the tank temperature, [K]

    Returns dy/dt = [F/V*(C_{A,in} - C_A) - k*C_A^2          ]
                   [F/V*(T_in - T) - k*C_A^2*HR/(rho*Cp) ]
    """
    F = 20.1      # L/min
    CA_in = 2.5   # mol/L
    V = 100.0     # L
    k0 = 0.15     # L/(mol.min)
    Ea = 5000     # J/mol
    R = 8.314     # J/(mol.K)
    Hr = -590     # J/mol
    T_in = 288    # K
    rho = 1.050   # kg/L

    # Assign some variables for convenience of notation
    CA = y[0]
    T = y[1]

    # Algebraic equations
    k = k0 * np.exp(-Ea / (R * T)) # L/(mol.min)
    Cp = 4.184 - 0.002 * (T - 273) # J/(kg.K)

    # Output from ODE function must be a COLUMN vector, with n rows
    n = len(y) # 2: implies we have two ODEs
    dydt = np.zeros((n))
    dydt[0] = F / V * (CA_in - CA) - k * CA ** 2
    dydt[1] = F / V * (T_in - T) - (Hr * k * CA ** 2) / (rho * Cp)
    return dydt
```

In [60]:

```
%matplotlib notebook

from scipy import integrate

# Start by specifying the integrator:
# use ``vode`` with "backward differentiation formula"
r = integrate.ode(tank).set_integrator('vode', method='bdf')

# Set the time range
t_start = 0.0
t_final = 45.0
delta_t = 0.1
# Number of time steps: 1 extra for initial condition
num_steps = int((t_final - t_start) / delta_t) + 1

# Set initial condition(s): for integrating variable and time!
CA_t_zero = 0.5
T_t_zero = 295.0
r.set_initial_value([CA_t_zero, T_t_zero], t_start)

# Create vectors to store trajectories
t = np.zeros(num_steps)
CA = np.zeros(num_steps)
temp = np.zeros(num_steps)

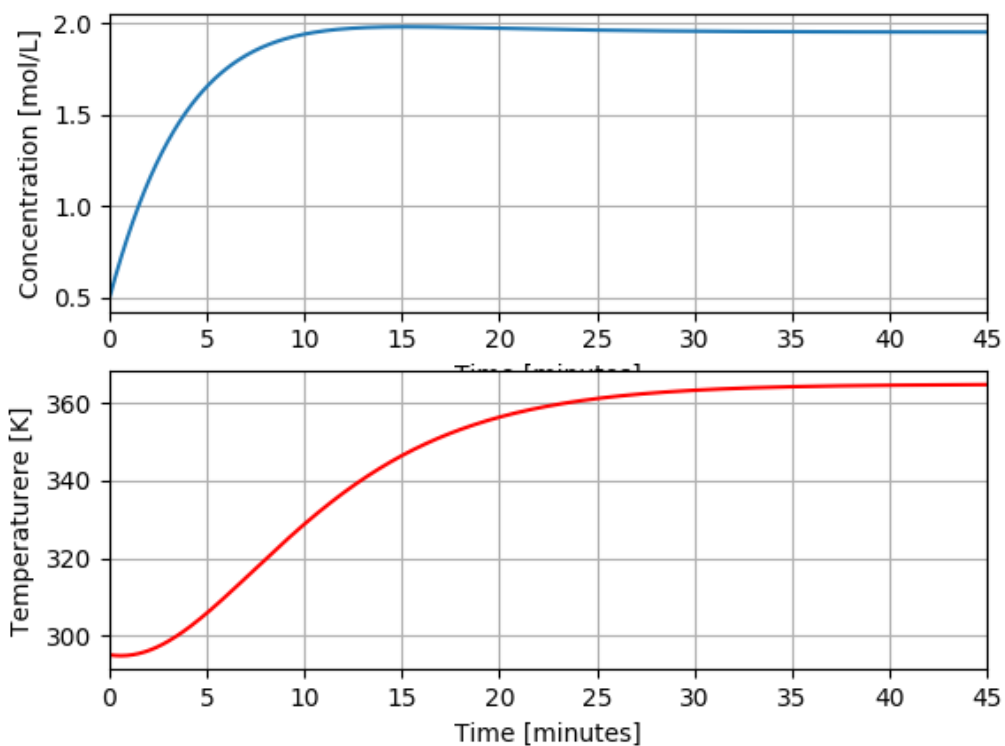
# Integrate the ODE(s) across each delta_t timestep
k = 0
while r.successful() and k < num_steps:
    # Store the results to plot later
    t[k] = r.t
    CA[k] = r.y[0]
    temp[k] = r.y[1]

    r.integrate(r.t + delta_t)
    k += 1
```

In [61]:

```
# All done! Plot the trajectories in two separate plots:
fig = plt.figure()
ax1 = plt.subplot(211)
ax1.plot(t[:k], CA[:k])
ax1.set_xlim(t_start, t_final)
ax1.set_xlabel('Time [minutes]')
ax1.set_ylabel('Concentration [mol/L]')
ax1.grid('on')

ax2 = plt.subplot(212)
ax2.plot(t[:k], temp[:k], 'r')
ax2.set_xlim(t_start, t_final)
ax2.set_xlabel('Time [minutes]')
ax2.set_ylabel('Temperaturere [K]')
ax2.grid('on')
```



Sympy

Symbolic calculus with Python

In [62]:

```
import sympy as sp
sp.init_printing()
x = sp.symbols('x')
f = sp.symbols('f', cls=sp.Function)
print(f(x))

sp.pprint(sp.Integral(sp.sqrt(1 / x), x))
diffeq = sp.Eq(f(x).diff(x, x) - 2 * f(x).diff(x) + f(x), sp.sin(x))
sp.pprint(diffeq)

sol = sp.dsolve(diffeq, f(x), dict=True)
sp.pprint(sol)
sol
```

f(x)

$$\int \sqrt{\frac{1}{x}} dx$$

$$f(x) - 2 \cdot \frac{d}{dx}(f(x)) + \frac{d^2}{dx^2}(f(x)) = \sin(x)$$

$$f(x) = (C_1 + C_2 \cdot x) \cdot e^x + \frac{\cos(x)}{2}$$

Out[62]:

$$f(x) = (C_1 + C_2 x) e^x + \frac{1}{2} \cos(x)$$

In [63]:

```
C1, C2 = sp.symbols('C1 C2')
sol.subs({x:2, C1:0, C2:3}).evalf()
```

Out[63]:

$$f(2) = 44.1262631753103$$