Modern scientific computing - problem set

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Contents

We present below a list of selected problems intended to challenge the skills of Scientific Python Programmers. Problems are sorted according to their level of complexity and the increasing number of required skills needed to solve them.

Try to solve first the simpler problems and go next through the more complex ones.

1 Prime numbers and the sieve of Erathostenes

Level: Basic (language,basic libraries)

The sieve of Erathostenes is a simple and famous algorithm for factoring prime numbers. You will find a nice explanation of the algorithm in Wikipedia.

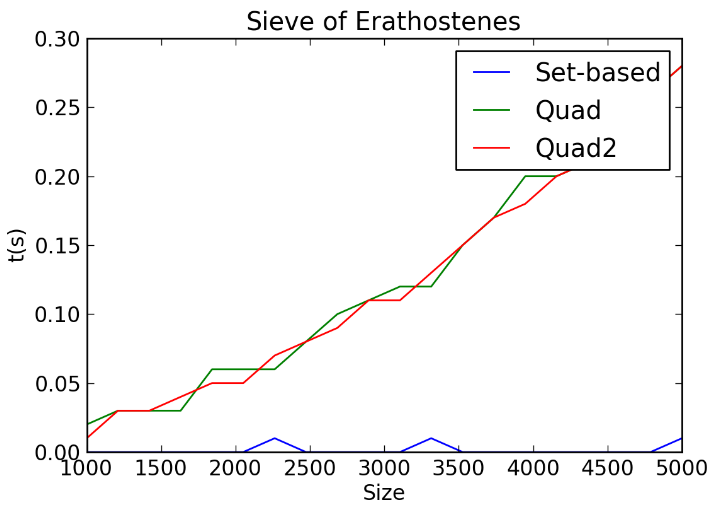
Try to implement it in Python, and think of different data structures you may use to do this.

Time the various implementations, do some analysis of the run times of each.

1.1 Solution

```
#!/usr/bin/env python
"""Simple example implementations of the Sieve of Erathostenes."""

__author__ = "Fernando Perez <Fernando.Perez@colorado.edu>"

import sys
import math

import numpy as np

def sieve_quad(nmax):
    """Return a list of prime numbers up to nmax.

    Naive, O(N^2) implementation using the Sieve of Erathostenes."""

    # Sanity checks
    assert nmax>1, "nmax must be > 1"
    if nmax == 2: return [2]

    # For nmax>3, do full sieve
    primes_head = [2]
    first = 3
    primes_tail = np.arange(first,nmax+1,2)
    while first <= round(math.sqrt(primes_tail[-1])):
        first = primes_tail[0]
        primes_head.append(first)
        non_primes = first * primes_tail
        primes_tail = np.array([ n for n in primes_tail[1:]
                                 if n not in non_primes ])

    return primes_head + primes_tail.tolist()


def sieve_quad2(nmax):
    """Return a list of prime numbers up to nmax.

    A slightly more readable implementation, still O(N^2)."""

    # Sanity checks
    assert nmax>1, "nmax must be > 1"
    if nmax == 2: return [2]

    # For nmax>3, do full sieve
    primes_head = [2]
    first = 3
    primes_tail = np.arange(first,nmax+1,2)
    while first <= round(math.sqrt(primes_tail[-1])):
        first = primes_tail[0]
        primes_head.append(first)
        non_primes = first * primes_tail
        primes_tail = np.array(list(set(primes_tail[1:])-set(non_primes)))
        primes_tail.sort()

    return primes_head + primes_tail.tolist()


def sieve(nmax):
    """Return a list of prime numbers up to nmax, using Erathostenes' sieve.

    This is a more efficient implementation than sieve_quad: we combine a
    set with an auxiliary list (kept sorted)."""

    # Sanity checks
    assert nmax>1, "nmax must be > 1"
    if nmax == 2: return [2]

    # For nmax>3, do full sieve
    primes_head = [2]
    first = 3

    # The primes tail will be kept both as a set and as a sorted list
    primes_tail_lst = range(first,nmax+1,2)
    primes_tail_set = set(primes_tail_lst)

    # optimize a couple of name lookups from loops
    tail_remove = primes_tail_set.remove
    head_append = primes_head.append
    sqrt = math.sqrt

    # Now do the actual sieve
    while first <= round(sqrt(primes_tail_lst[-1])):
        # Move the first leftover prime from the set to the head list
        first = primes_tail_lst[0]
        tail_remove(first)  # remove it from the set
        head_append(first) # and store it in the head list

        # Now, remove from the primes tail all non-primes.  For us to be able
        # to break as soon as a key is not found, it's crucial that the tail
        # list is always sorted.
        for next_candidate in primes_tail_lst:
            try:
                tail_remove(first*next_candidate)
            except KeyError:
                break

        # Build a new sorted tail list with the leftover keys
        primes_tail_lst = list(primes_tail_set)
        primes_tail_lst.sort()

    return primes_head + primes_tail_lst

if __name__ == '__main__':
    # A simple test suite.
    import unittest

    # Make the generic test NOT be a subclass of unittest.TestCase, so that it
    # doesn't get picked up automatically.  Each subclass will specify an
    # actual sieve function to test.
    class sieveTestBase:

        def test2(self):
            self.assert_(self.sieve_func(2)==[2])

        def test100(self):
            primes100 = [2, 3, 5, 7, 11, 13, 17, 19, 23, 29, 31, 37, 41,
                         43, 47, 53, 59, 61, 67, 71, 73, 79, 83, 89, 97]
            self.assert_(self.sieve_func(100)==primes100)

    # These subclasses define the actual sieve function to test.  Note that it
    # must be set as a staticmethod, so that the 'self' instance is NOT passed
    # to the called sieve as first argument.
    class sieveTestCase(sieveTestBase,unittest.TestCase):
        sieve_func = staticmethod(sieve)

    class sieve_quadTestCase(sieveTestBase,unittest.TestCase):
        sieve_func = staticmethod(sieve_quad)

    class sieve_quad2TestCase(sieveTestBase,unittest.TestCase):
        sieve_func = staticmethod(sieve_quad2)

    # Other code for demonstration purposes
    def time_rng(fun,nrange,ret_both=0,verbose=1):
        """Time a function over a range of parameters.

        Returns the list of run times.

        The function should be callable with a single argument: it will be
        called with each entry from nrange in turn.

        If verbose is true, at each step the value of nrange and time for the
        call is printed."""

        def time_n(n):
            "Simple closure for local timings"
            import time
            t0 = time.clock()
            fun(n)
            return time.clock() - t0

        times = []
        write = sys.stdout.write
        flush = sys.stdout.flush
        for n in nrange:
            t = time_n(n)
            if verbose:
                if verbose==1:
                    write('.')
                elif verbose>1:
                    print n,t
                flush()
            if t==0: t = 1e-9
            times.append(t)

        if ret_both:
            return nrange,times
        else:
            return times

    def time_sieves():
        "simple timing demo"

        def plot_sieve(sieve,label):
            r,t = time_rng(sieve,rng,1,2)
            plt.plot(r,t,label=label)

        from matplotlib import pyplot as plt

        rng = np.linspace(1000,5000,20).astype(int)
        plt.figure()
        plt.title('Sieve of Erathostenes')
        plt.xlabel('Size')
        plt.ylabel('t(s)')

        plot_sieve(sieve,'Set-based')
        plot_sieve(sieve_quad,'Quad')
        plot_sieve(sieve_quad,'Quad2')

        plt.legend()
        plt.show()

    # This must be called LAST, because no code after it will be seen.
    print "To see timings comparison, call time_sieves()"
    unittest.main()
```

After calling `time_sieves()`, we can see how much impact different data structure choices can have on algorithm run time:



2 Monte Carlo integration

Level: Basic (language,basic libraries)

Compute π via Monte Carlo integration. To do this, think of a function whose integral is related to π (e.g. $\int_0^1 1/(1+x^2)dx$), and then compute this integral via Monte Carlo integration.

Try several different functions and compare.

2.1 Solution

```
#!/usr/bin/env python
"""Simple generation of pi via MonteCarlo integration.

We compute pi as the area of a unit circle, and we compute this area by
integration:

A = pi = 4*int_0^1{sqrt(1-x^2)}

This integral is then done via MonteCarlo integration.

In this example, we do it both in pure Python and then by calling weave.inline
to speed up the loop.
"""

import math
import random

import numpy as np

from scipy import weave


def v1(n = 100000):
    """Approximate pi via monte carlo integration"""

    rand = random.random
    sqrt = math.sqrt
    sm   = 0.0
    for i in xrange(n):
        sm += sqrt(1.0-rand()**2)
    return 4.0*sm/n


def v2(n = 100000):
    """Implement v1 above using weave for the C call"""

    support = "#include <stdlib.h>"

    code = """
    double sm;
    float rnd;
    srand(1); // seed random number generator
    sm = 0.0;
    for(int i=0;i<n;++i) {
        rnd = rand()/(RAND_MAX+1.0);
        sm += sqrt(1.0-rnd*rnd);
    }
    return_val =  4.0*sm/n;"""
    return weave.inline(code,('n'),support_code=support)

if __name__ == '__main__':

    # Monte Carlo Pi:
    print 'pi is:', math.pi
    print 'pi - python:',v1()
    print 'pi - weave :',v2()

    from timeit import timeit
    tpy = timeit('v1()','from montecarlo_pi import v1', number=10)/10.0
    tw = timeit('v2()','from montecarlo_pi import v2', number=10)/10.0
    print 'Python time %.2g s' % tpy
    print 'Weave time %.2g s' % tw
    print 'Weave speedup:',tpy/tw
```

This code includes a weave-enabled version of the computation, to illustrate how certain cases can be easily sped up with very little effort.

3 Cellular automata

Level: Basic (language, basic libraries, plotting)

Compute the evolution of a 2D Cellular Automaton (CA) given a random initial state, a simple set of cell update rules and a given boundary condition.

As an example create one of the most famous CA, The Life Game:

1. Generate a 2D matrix of integer values between 0 and 3 (0: dead cell, 1: recently born, 2: alive, 3: recently dead.)
2. Update the state of each cell using the following conditions:

   1. If a cell is dead but there are exactly 3 neighbor cells alive, she will born (passes from state 0 to state 1)

   2. If a cell is alive and there are 2 or 3 neighbor cells alive she stays alive (passes from state 1 to 2 or stays in state 2), otherwise it dies (passes from state 2 to 3).
3. Use a *cold* boundary condition, i.e. all the cells beyond the boundary of the CA are dead.
4. Plot the state of the CA on each step.

Bonus: Create an animation of the evolution of the Automaton.

Bonus: Change the boundary condition. Options are: *hot* boundary condition (all the cells outside are alive), periodic boundary condition or a reflecting boundary condition.

References: http://en.wikipedia.org/wiki/Cellular_automaton

4 Simple fitting

Level: Medium (scientific libraries, plotting)

Test different methods of fitting using a signal with known source.

1. Generate data pairs (x, y) in the range $x \in [0, 4]$ from the target function:

$$y(x) = a\exp(\alpha x) + k$$

   Using the following choice of constants: $a = 2, \alpha = -0.75, k = 0.1$.
2. Add zero-mean gaussian noise to y, with amplitude 0.1 to create a noisy version of the signal.
3. Fit the noisy data using the following methods: least-square fit to the analytical form, splines (from `scipy.interpolate`), polynomial fit (from `numpy`) of orders 0, 1 and 2.
4. Plot the data and the results from the fitting procedures and Compare graphically the fitting methods.

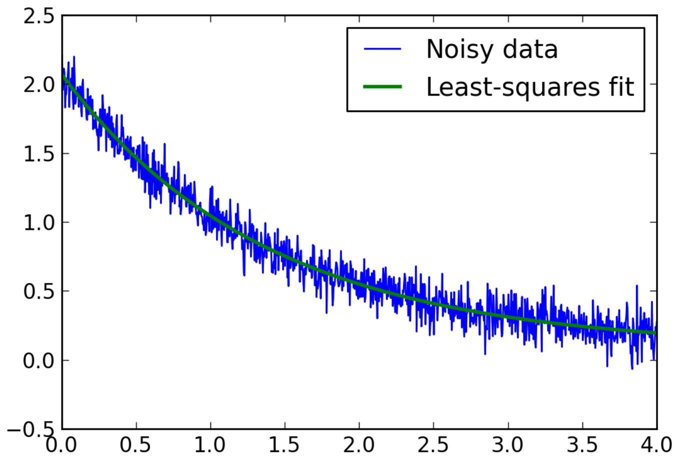
4.1 Solution

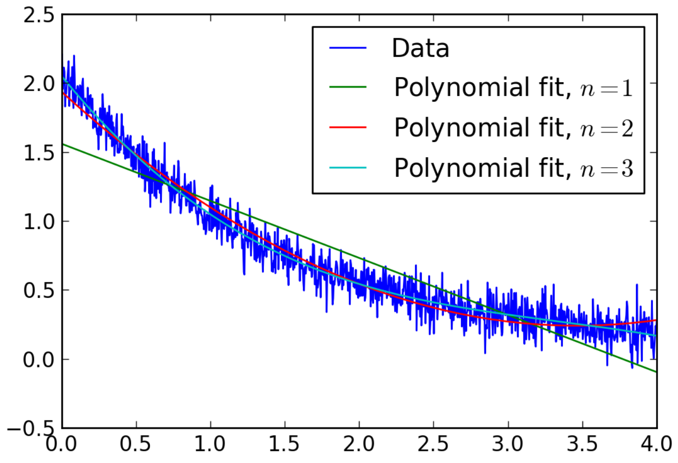
```
#!/usr/bin/env python
"""Simple data fitting and smoothing example"""

from numpy import exp,arange,array,linspace
from numpy.random import normal

from scipy.optimize import leastsq
from scipy.interpolate import splrep,splev
```

```
import numpy as np
import matplotlib as mpl
import matplotlib.pyplot as plt

def func(pars):
    a, alpha, k = pars
    return a*exp(alpha*x_vals) + k

def errfunc(pars):
    """Return the error between the function func() evaluated"""
    return y_noisy - func(pars)  #return the error

# Use globals for the x values and true parameters
pars_true = array([2.0, -.75, 0.1])
x_vals = linspace(0, 4, 1000)

# some pseudo data; add some noise
y_noisy = func(pars_true) + normal(0.0, 0.1, x_vals.shape)

# the intial guess of the params
guess = 1.0, -.4, 0.0

# now solve for the best fit paramters
best, mesg = leastsq(errfunc, guess)

print 'Least-squares fit to the data'
print 'true', pars_true
print 'best', best
print '|err|_l2 =',np.linalg.norm(pars_true-best)

# scipy's splrep uses FITPACK's curfit (B-spline interpolation)
print
print 'Spline smoothing of the data'
sp = splrep(x_vals,y_noisy)
smooth = splev(x_vals,sp)
print 'Spline information (see splrep and splev for details):',sp

# Polynomial fitting
def plot_polyfit(x,y,n,fignum=None):
    """ """
    if fignum is None:
        fignum = plt.figure().number
        plt.plot(x,y,label='Data')

    fit_coefs = np.polyfit(x,y,n)
    fit_val = np.polyval(fit_coefs,x)
    plt.plot(x,fit_val,label='Polynomial fit, $n=%d$' % n)
    plt.legend()
    return fignum

# Now use pylab to plot
```

```
plt.figure()
plt.plot(x_vals,y_noisy,label='Noisy data')
plt.plot(x_vals,func(best),lw=2,label='Least-squares fit')
plt.legend()
plt.figure()
plt.plot(x_vals,y_noisy,label='Noisy data')
plt.plot(x_vals,smooth,lw=2,label='Spline-smoothing')
plt.legend()

fignum = plot_polyfit(x_vals,y_noisy,1)
plot_polyfit(x_vals,y_noisy,2,fignum)
plot_polyfit(x_vals,y_noisy,3,fignum)

plt.show()
```

The least-squares and polynomials fits should look like this:





5 Fractals

Level: Medium (plotting)

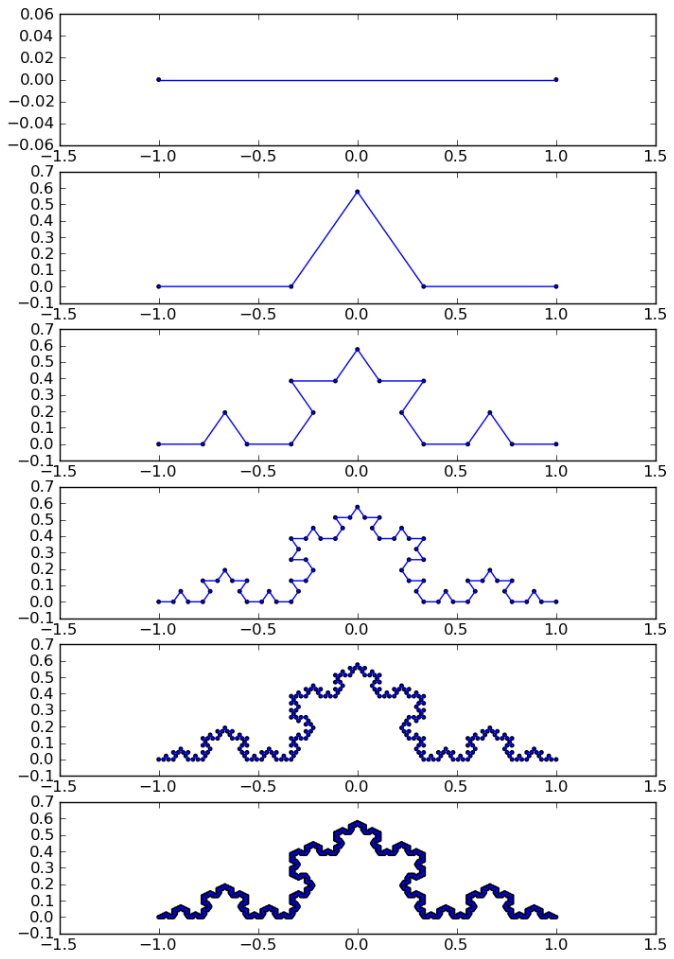
A simple ilustration of fractal curve is the von Koch curve K.

$$K = S_\infty \tag{1}$$

This curve is constructed by the following procedure mentioned below: In the iteration S_0 we take a line segment of longitud L and split it in three equal parts and the middle one is substracted. Then we replace the missing segment with the other two sides of an equlateral triangle.

The remaining iterations consist in repeat the procedure for each one or the segments in the previous approximation.

Write a python script to plot the six first iteration in the construction of the von Koch curve as ilustrated in the figure.



6 The least action principle

Level: Medium (scientific libraries, algorithms)

From: http://www.eftaylor.com/software/ActionApplets/LeastAction.html (With Java applets)

Java source code at: http://www.eftaylor.com/leastaction.html

Throw an apple vertically upward from the ground (zero height). We demand that 3 seconds later the apple return to our hand at the same height (zero) from which we launched it. What is the motion of this apple between the events of launch and catch? At what height can the apple be found at any given time? Or to express the question more technically: What is the worldline of the apple between launch and catch? We use the principle of least action to find answers to these questions.

$$S \equiv \int_{\text{entire worldline}} L\,dt = \int_{\text{entire worldline}} (T - V)\,dt$$

The principle of least action defines the action S for motion along a worldline between two fixed events:

Here L is called the Lagrangian. In simple cases the Lagrangian is equal to the difference between the kinetic energy T and the potential energy V, that is, $L = T\breve{}V$. In this interactive document we will approximate a continuous worldline with a worldline made of straight connected segments. The computer then multiplies the value of $(T\breve{}V)$ on each segment by the time lapse t for that segment and adds up the result for all segments, giving us an approximate value for the action S along the entire worldline. Our task is then to move the connected segments of the worldline so that they result in the minimum total value of the action S.

In the following we assume a mass of 0.2 kilogram for the apple.

Try to obtain a plot similar to the obtained in "Display #2: Automatic hunting for worldline of least action", when the button `Hunt` is clicked:

7 Sequence alignment

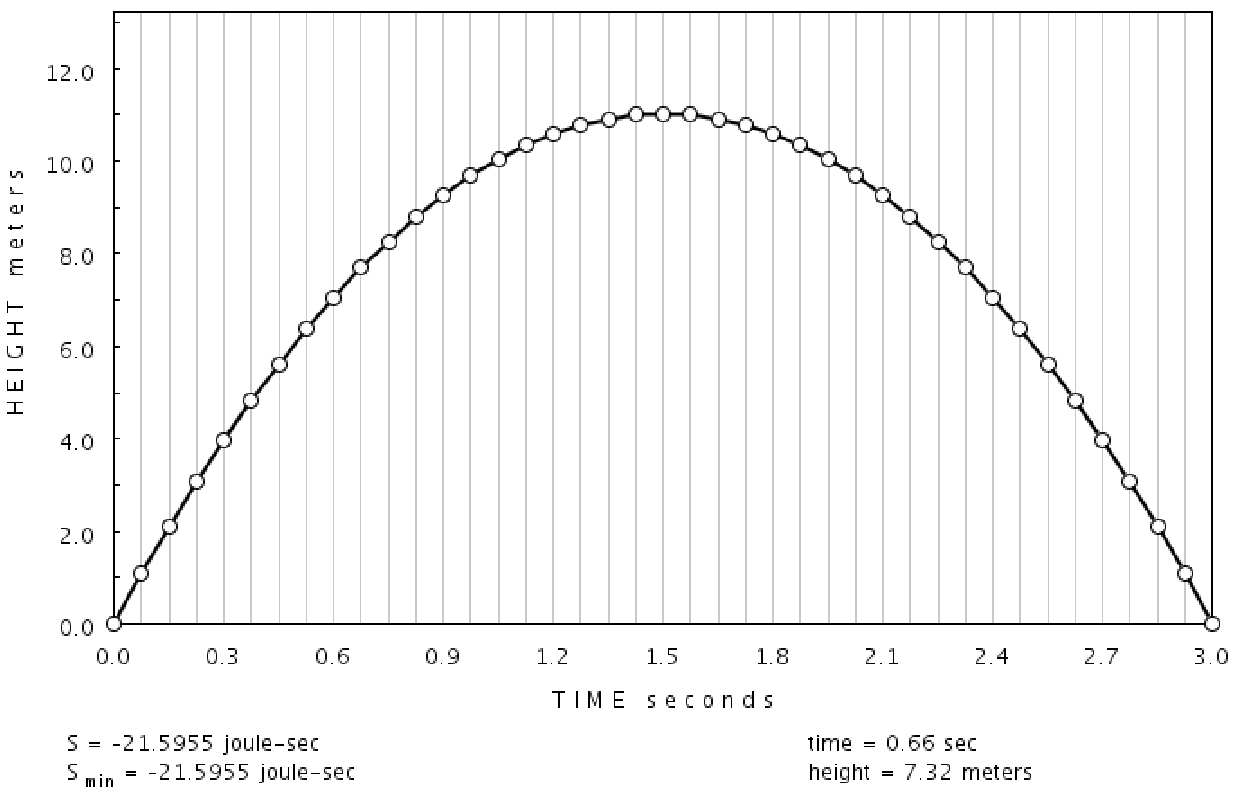
Level: Advanced (algorithm, language)

Write a python Script to compute the global sequence alignment of two nucleotide sequences using a simple implementation of the Needleman-Wunsch algorithm.

1. Generate two random sequences of a given length using letters in the set $\{A, G, C, T\}$ (e.g. AGTGAC, TACGGA)
2. Construct a simple *similarity function* $S(A, B)$:

$$S(A,B) = \begin{cases} w_M & \text{if } A = B \\ w_U & \text{if } A \neq B \end{cases}$$

   Where A and B are any letters in the symbols set and $w_M = 10$ $w_U = -5$ (gap scoring.) This function is used to score the matches between nucleotides in the sequences.



3. Construct the *F-matrix* of the sequences, i.e. the matrix which contains information about the matching of every single character in both sequences:

$$F_{ij} = \begin{cases} w_D & \text{if } i = 0 \text{ or } j = 0 \\ max(F_{i-1,j-1} + S(A_i, B_j), F_{i,j-1} + w_D, F_{i-1,j} + w_D) & \text{otherwise} \end{cases}$$

   Where A_i is the i-th letter in the sequence A and $w_D = -5$

4. The F-matrix has the instructions to build the final alignment. For the example sequences A=AGTGAC, B=TACGGA the F-matrix looks like:

$$F = \begin{pmatrix} -5 & -5 & -5 & -5 & -5 & -5 \\ -5 & -10 & -10 & 5 & 5 & 0 \\ -5 & -10 & -15 & 0 & 0 & 0 \\ -5 & -10 & -15 & -5 & 10 & 5 \\ -5 & 5 & 0 & -5 & 5 & 20 \\ -5 & 0 & 15 & 10 & 5 & 15 \end{pmatrix}$$

   To build the aligned sequences A', B', start in the lowermost, rightmost component of the matrix. Compare that element with their neighbors: diagonal $(i-1, j-1)$, left $(i, j-1)$ and up $(i-1, j)$. Find the larger value among them and *move* in that direction.

   If your last movement was in the diagonal direction, add to aligned sequences the respective character in the original sequences.

   If you move up, add to the aligned sequence A' the respective character of A and to B' add a symbol '-' (insertion or deletion symbol).

Finally if you move to left, add to the aligned sequence B' the respective character in B and put a '-' symbol in A'.

Repeat this procedure until you reach the first line or column.

With the sequences provided above the final aligned sequences are:

–GTGAC

TAG-GA-

Bonus: Try to measure the aligning time of long sequences and to figure out the way as the time increases with the length of the sequences.

Bonus: Try changing the values of the gap-scoring (w parameters).

A detailed but slightly different explanation of the algorithm could be found in the Wikipedia article: http://es.wikipedia.org/wiki/Algoritmo_Needleman-Wunsch.

8 Command line calculator

Level: Advanced (algorithm, language, scientific libraries)

Make a python program that works as a command line calculator, `pycalc` in the same spirit that the beloved UNIX program `bc`.

The program should work as in the following examples:

```
$ pycalc "2*pi^2*sin(0.7)/atan(60)"
8.1822869377000984
```

Note the use of ^ instead of `**`. The calculator should use by default the `math` library.

When dealing with complex numbers the python calculator should import the `cmath` library:

```
$ pycalc -c "2*pi^2*asin(2+3j)/atan(60)"
(7.247930188215947+25.191239093226159j)
```

where the `-c` options allows to work with complex numbers.

Bonus 1: Deal with rationals and integers:

```
$ pycalc 2/3+8/5
34/15
```

Bonus 2: Input from pipes:

```
$ pycalc 2/3+8/5 | pycalc -r
2.26666666667
```

where the `-r` option forces the numbers in expression to be real.

8.1 Solution

```
#!/usr/bin/env python
# -*- coding: utf-8 -*-
import re
import sys
import commands
from math import *

from optparse import OptionParser
#mensaje de --help
usage = u'''%prog [Options] EXPR
where EXPR is the mathematical expresion to evaluated.

Examples:
 $ pycalc "2*pi^2*sin(0.7)/atan(60)"
   8.1822869377000984

 $ pycalc 2/3+8/5
   34/15

 $ pycalc 2/3+8/5 | pycalc -r
   2.26666666667'''

parser=OptionParser(usage=usage)
parser.add_option("--d16", action="store_true", dest="d16",help="print with 16 digits")
parser.add_option("-r", action="store_true", dest="noreal",help="force all number to be rea
parser.add_option("-c", action="store_true", dest="cpl",help="Use complex math functions")
(options,args)=parser.parse_args() #by default it uses sys.argv[1:]

if options.cpl:
    from cmath import *

expr=''
if args:
    tmp = args[0:]
    for i in args:
        expr=expr+i #expr is an string
else: #
    expr=sys.stdin.readlines()[0] # expr is an string, further work to use all the lines

result=expr.replace('^','**')
#Try to change integer to real
if options.noreal:
    result=re.sub(r'(\d+)',r'\1.',result)
    result=result.replace('..','.')
    result=re.sub(r'(\d+\.\d+)\.',r'\1',result)
    result=re.sub(r'(\d+\.[Ee][+-]\d+)\.',r'\1',result)

#integer calculations
if not re.search('[a-z\.A-Z]',result,re.I):
    import sympy
    result=re.sub(r'([0-9]+)',r'sympy.Integer(\1)',result)
```

```
eresult=eval(result)
if options.d16:
    print '%.16f' %(eresult)
else:
    print eresult
```

9 Tree methods for sumations

Level: Advanced (algorithm, language, Object Orientated Programming)

One of the most common numerical tasks in problems involving the simulation of dynamical processes in N-body systems is the computation of large number of summations with the form:

$$f_i = \sum_{j=1}^{j=N} g_{ij}$$

One example is the computation of a long-range force exerted on a particle by the rest of particles in a given physical system.

To compute the evolution of that kind of systems $O(N^2)$ computations of the g_{ij} terms are required and with a large value of N the computational cost is huge.

One of the most clever solution of this problem is the so-called *tree-method for summation*. In that method the value of g_{ij} corresponding to distant particles are summed up by constructing a hierarchical structure of nested cells (tree).

The tree is constructed using the following procedure:

1. Divide the initial *volume* in 2^D equal regions ($D = 1, 2, 3$ is the number of space dimensions of the problem)
2. Compute the physical properties of each cell: total mass or total charge, gravitational or electrical multipole momenta, etc.
3. Store the geometrical paramters of each cell: center of mass or charge, dimensions, position of its vertices.
4. Store a list of the particles contained on each cell.
5. Tag the cell with an identification number.
6. Store the tags of the father cell (0 for the original volume) and a list of the tags of the child cells if there is any (see next step).
7. Repeat 1-6 for every child cell that contains more than 1 particle.

The summation for each particle is performed in the following way:

1. Loop on the tree starting in the highest level (tag 1, 2, ... skip the 0 level)
2. For each cell compute the distance from the centroid to the particle (d).

3. If $s/d < 0.5$, where s is the size of the cell compute the force exerted by the whole cell on the particle.
4. Else descend on the child cells and repeat from step 2.

At the end the computation of all the summations for the N particles is performed in $O(NlogN)$ instead of the original $O(N^2)$.

Write a python script to compute the gravitational force on each particle of a system composed by N randomly distributed particles in a 1D line and using a tree-method to compute the summation.

The specific gravitational force on particle i exerted by another particle is given by:

$$f_i = -\frac{M}{R_i^3}\vec{R}_i$$

Where $R_i = \vec{r_i} - \vec{r}$, M and $\vec{r}$ is the mass parameter and position of the other particle.

Bonus: Compare the time required to perform the operation using the direct summation and the tree mathod.

Bonus: Write the program to perform the summation in 2 and 3D.

In addition to the problems listed here, you should study the Scipy Cookbook (http://www.scipy.org/Cookbook), where a lot of very good problems are presented with full solutions.