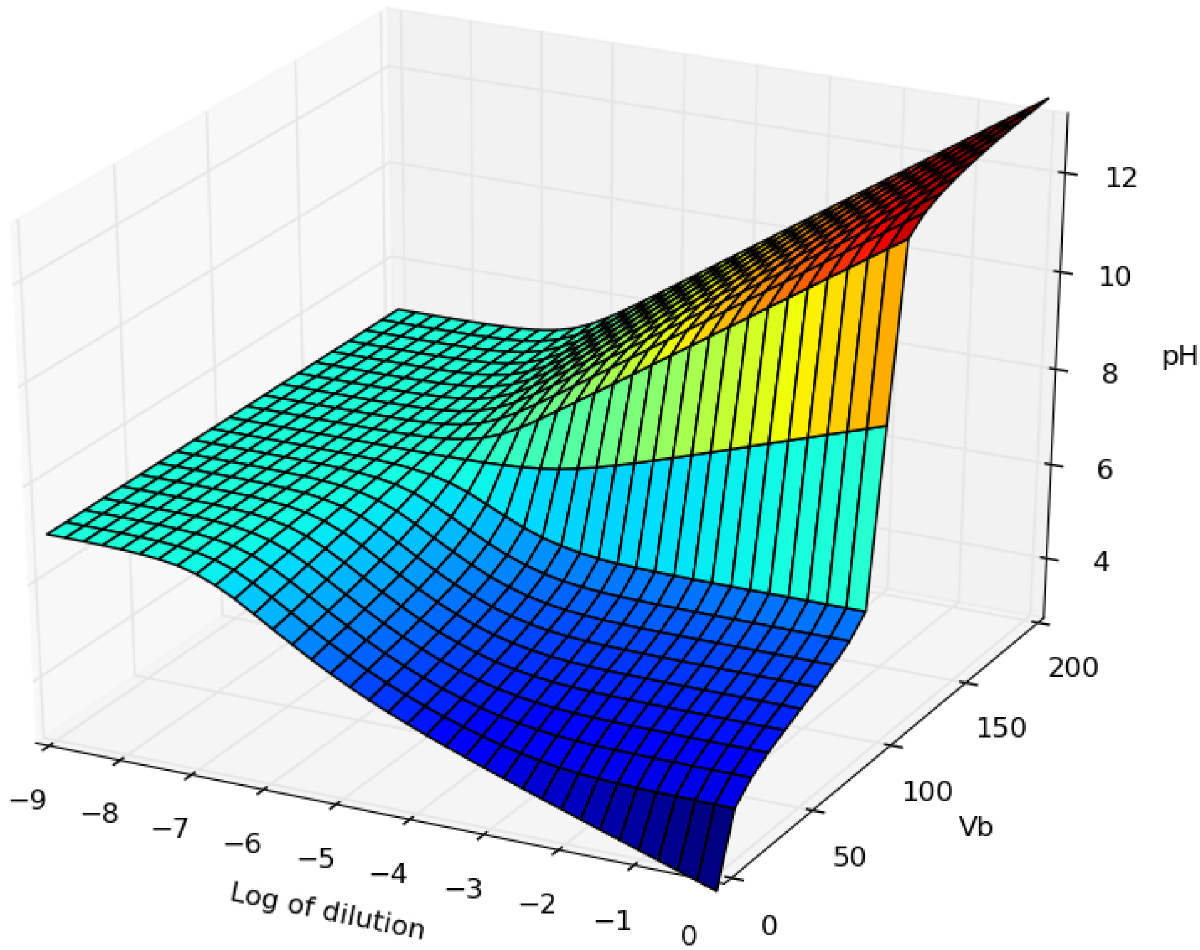
Cas d'un acide en fonction d'un ajout de base et d'une dilution globale : cf. cet article

pH-3D_topo-01.py

```
#! /usr/bin/env python
# -*- coding: utf-8 -*-
"""
Use of numpy polynomes to compute pH of weak acid and strong base

3D topographic surface generation in the same conditions as
the following paper :
3-D Surface Visualization of pH Titration “Topos”:
Equivalence Point Cliffs, Dilution Ramps, and Buffer Plateaus"
Garon C. Smith, Md Mainul Hossain and Patrick MacCarthy
J. Chem. Educ., 2014, 91 (2), pp 225–231   DOI: 10.1021/ed400297t
see fig here : http://pubs.acs.org/doi/abs/10.1021/ed400297t

Python code under GPLv3 GNU General Public License
http://www.gnu.org/licenses/gpl-3.0.html

Didier Villers, UMONS
http://dvillers.umons.ac.be/blog/contact/
"""
import numpy as np
import numpy.polynomial.polynomial as poly
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import *  # Axes3D
from matplotlib import cm           # Colors

def pH_monoprotic_acid(log10dil,Vb):
    # this Python function operate on numbers and cannot be applied on
ndarrays due to the polynomial roots search
    dil=10**log10dil
    Ca=Ca0*dil
    Cb=Cb0*dil
    #
http://docs.scipy.org/doc/numpy/reference/generated/numpy.polynomial.po
lynomial.polyroots.html#numpy.polynomial.polynomial.polyroots
    #
http://docs.scipy.org/doc/numpy/reference/generated/numpy.polynomial.po
lynomial.polyval.html#numpy.polynomial.polynomial.polyval
    p=np.array([-Ka*Kw,-Kw-Ka*(Ca*Va-
Cb*Vb)/(Va+Vb),Ka+(Cb*Vb)/(Va+Vb),1])
    x=poly.polyroots(p)
    return float(-np.log10(x[np.where(abs(x-27.5)<27.5)]))  # only
significant [H+] is returned

Ka=1.75E-5 # acid constant (acetic acid)
Kw=1.E-14 # water product
Ca0=1. # acid concentration
Cb0=1. # base concentration
```

```
Va=0.1 # volume of acid
Vb=0. # volume of added base
log10dil=0
print(pH_monoprotic_acid(log10dil,Vb)) # sample call

fig = plt.figure()
ax = Axes3D(fig)
X,Y = np.linspace(-9.,0.,36),  np.linspace(0.,200.,21)
print(type(X), X.ndim, X.shape, X.dtype)
print(type(Y), Y.ndim, Y.shape, Y.dtype)
Xc, Yc = np.meshgrid(X, Y)
Z = Xc+Yc # just to create Z
print(type(Xc), Xc.ndim, Xc.shape, Xc.dtype)
print(type(Yc), Yc.ndim, Yc.shape, Yc.dtype)
print(type(Z), Z.ndim, Z.shape, Z.dtype)
print(range(len(X)))
for ix in range(len(X)):
    for iy in range(len(Y)):
        # print ix, iy,X[ix],Y[iy],pH_monoprotic_acid(X[ix],1E-3*Y[iy])
        Z[iy][ix] = pH_monoprotic_acid(X[ix],1E-3*Y[iy])

ax.plot_surface(Xc,Yc,Z, rstride=1,cstride=1,cmap=cm.jet)
ax.set_xlabel('Log of dilution')
ax.set_ylabel('Vb')
ax.set_zlabel('pH')
plt.show()
```

La figure obtenue avec la librairie 3D de MatPlotlib peut être manipulée (zoom, rotations). En voici une image correspondant à la figure de l'article référencé dans Journal of Chemical Education :



- 3-D Topo Surface Visualization of Acid–Base Species Distributions: Corner Buttes, Corner Pits, Curving Ridge Crests, and Dilution Plains Garon C. Smith and Md Mainul Hossain, J. Chem. Educ., 2017, 94 (5), pp 598–605 DOI: 10.1021/acs.jchemed.6b00682