APN_Conductivity_SDS_V1b

March 17, 2018

1 Determination of the critical micelle concentration of Sodium dodecyl sulfate (SDS) in water

Example of a nonlinear curve fit of Surfactant Conductivity Data The fit functions are based on the "APN"-model for the concentration of surfactants near the cmc

More details on our web page http://www.usc.es/fotofqm/en/units/single-molecule-fluorescence/concentration-model-surfactants-near-cmc

A Model for Monomer and Micellar Concentrations in Surfactant Solutions. Application to Conductivity, NMR, Diffusion and Surface Tension data Wajih Al-Soufi, Lucas Piñeiro, Mercedes Novo, Journal of Colloid and Interface Science 2012, 370, 102–110 DOI: 10.1016/j.jcis.2011.12.037

Python code based on "Simple nonlinear least squares curve fitting in Python", http://www.walkingrandomly.com/?p=5215

V1 - 2018/04/18

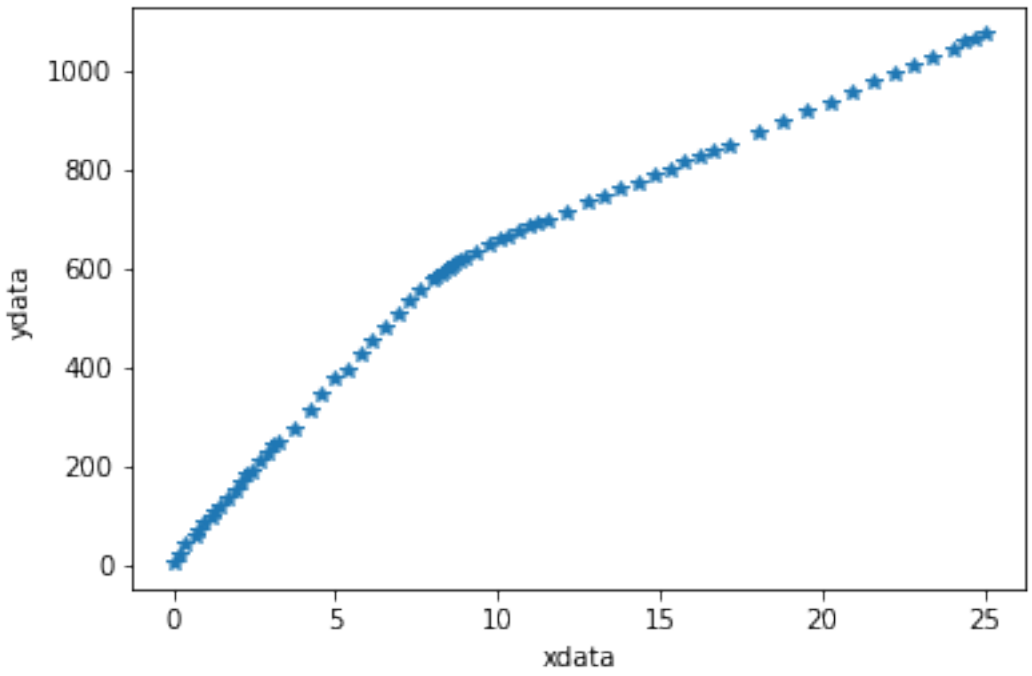
```
In [1]: import numpy as np
        import math
        import matplotlib.pyplot as plt
        from scipy.optimize import curve_fit
        import scipy.special as sc
```

1.0.1 Conductivity data:

xdata: Total Surfactant concentration [S]0(mM) ydata: Surfactant Conductivity Data (uS/cm)

```
In [2]: xdata = np.array([0.00, 0.20, 0.40, 0.69, 0.79, 0.98, 1.17, 1.27, 1.46, 1.64, 1.92, 2.11
        ydata = np.array([3.5, 18.7, 38.3, 59.9, 67.6, 85, 97.1, 107.6, 116, 131.8, 150.2, 165.1
```

```
In [3]: plt.plot(xdata,ydata,'*')
        plt.xlabel('xdata')
        plt.ylabel('ydata');
```



1.0.2 Function definition "APN"-Model

APNS1(cS0,cmc,r) Takes [S]0 and calculates the monomeric concentration [S1] as function of the cmc and the relative transition width r

```
In [4]: def APNS1(cS0,cmc,r):
            s0 = cS0/cmc;
            pi = math.pi;
            A=2/(1+np.sqrt(2/pi)*r*np.exp(-1/(2*r*r))+sc.erf(1/np.sqrt(2)/r));
            cS1=cmc*(1-(A/2)*(np.sqrt(2/pi)*r*np.exp(-(s0-1)**2/(2*r*r))+(s0-1)*(sc.erf((s0-1)/(
            return cS1
```

APNConductivity(cS0,cmc,r,a,b,c) Takes [S]0 and calculates the electric conductivity as function of the cmc, the relative transition width r, the slopes a and b, and the solvent conductivity c = s.

```
In [5]: def APNConductivity(cS0,cmc,r,a,b,c):
            cS1 = APNS1(cS0, cmc, r)
            cSm = cS0 - cS1
            return a * cS1 + b * cSm + c
```

1.0.3 Nonlinear curve fit

Initial parameter values (cmc,r,a,b,c)

```
In [6]: p0=(8.0,0.1,70.0,30.0,10.0)

In [7]: popt, pcov = curve_fit(APNConductivity, xdata, ydata,p0) # fit
        psd = np.sqrt(np.diagonal(pcov)) # calculate parameter standard deviations
        print(popt) # optimized parameter values
        print(psd) # parameter standard deviations

[  8.18798535   0.12737425  72.54979584  27.72754611  10.73056648]
[ 0.03828131  0.00908576  0.26777009  0.09614226  0.88426139]
```

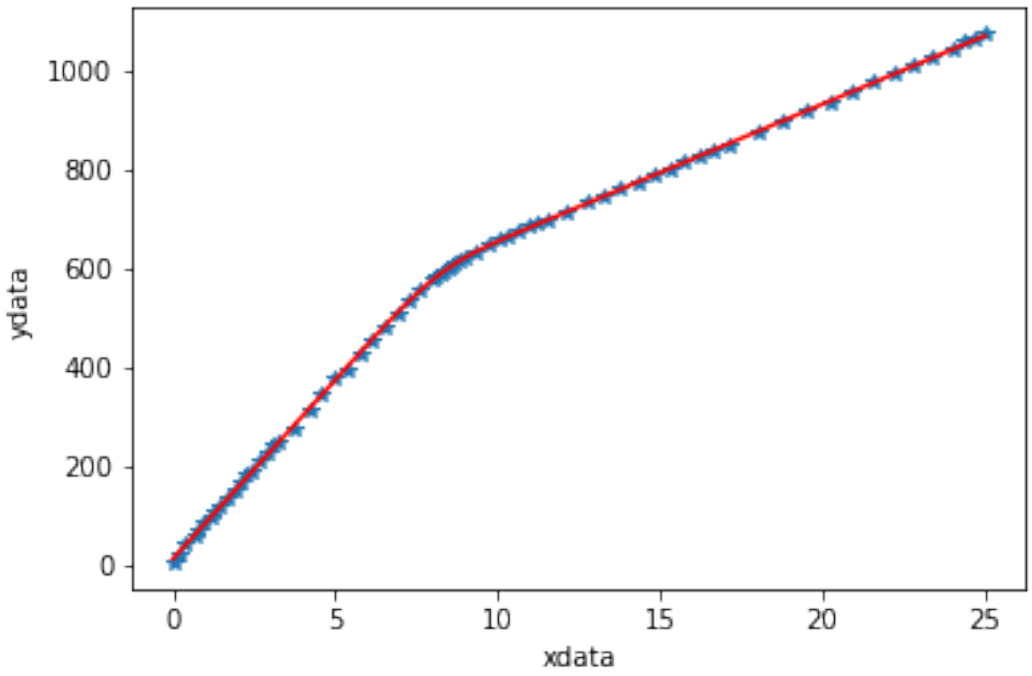
Results

```
In [8]: print('cmc = %0.4g ś %0.2g'%(popt[0],psd[0]), '\nr = %0.4g ś %0.2g'%(popt[1],psd[1]))

cmc = 8.188 ś 0.038
r = 0.1274 ś 0.0091
```

```
In [9]: residuals = ydata - APNConductivity(xdata,*popt)
        fres = sum(residuals**2)
        fres #Sum of squared residuals

Out[9]: 432.14136281923504
```

Plot result

```
In [10]: curvex=np.linspace(xdata[0],xdata[-1],100)
         curvey=APNConductivity(curvex,*popt)
         plt.plot(xdata,ydata,'*')
         plt.plot(curvex,curvey,'r')
         plt.xlabel('xdata')
         plt.ylabel('ydata');
```



In [11]:
```
plt.plot(xdata,residuals,'*')
plt.xlabel('xdata')
plt.ylabel('ydata');
```