Problem Set 9 Statistical Methods

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1 Question 1

1. Covariance of y_1 and y_2 . Note that y_2 can be rewritten

$$y_2 = \frac{1}{m} \sum_{j=n-c+1}^{m+n-c} x_j = \frac{1}{m} \sum_{j=1}^{m} x_j$$

So we have

$$cov[y_1, y_2] = E\left[\left(\frac{1}{n}\sum_{i=1}^n x_i\right)\left(\frac{1}{m}\frac{1}{m}\sum_{j=1}^m x_j\right)\right] - \mu^2$$

$$= \frac{1}{nm}\left[(nm - n - m)\mu^2 + \mu^2(n + m) + c\sigma^2\right] - \mu^2$$

$$= \frac{c\sigma^2}{nm}$$

This method is adapted from Glen cowan's book equation 5.13. The difference arises from the c term which is introduced as an overlap between the observations. I was unsure how to calculate this for the given summation in the question, I just transformed them into more manageable ones. I haven't shown the equality between the different summations for y_2 however this is trivial.

From this we can also see that the correlation coefficient is

$$\rho = \frac{c}{\sqrt{nm}}$$

$$\sigma_1 = \frac{\sigma}{\sqrt{n}}$$

$$\sigma_2 = \frac{\sigma}{\sqrt{m}}$$

2. The weighted average for correlated results (section 7.6 GC) is

$$\hat{\lambda} = wy_1 + (1 - w)y_2$$

Where the weights w is

$$w = \frac{\sigma^2 - \rho \sigma_1 \sigma_2}{2\sigma_2 - 2\rho \sigma_1 \sigma_2} = \frac{1}{2}$$

So we have

$$\hat{\lambda} = \frac{1}{2}y_1 + \frac{1}{2}y_2 = \frac{y_1 + y_2}{2}$$

The variance is given by

$$V[\hat{\lambda}] = \frac{1}{\frac{1}{V[y_1]} + \frac{1}{V[y_2]}} = \frac{\sigma^2}{2}$$

3. The weighted w_i are given by

$$\frac{\sum_{i,j=1}^{N} (V^{-1})_{ij}}{\sum_{k,l=1}^{N} (V^{-1})_{kl}}$$

The weights will always be positive because

$$\frac{\sigma_1}{\sigma_2} = \sqrt{\frac{m}{n}}$$

So the correlation coefficient will always be less than or equal to the difference between the variances. The average will always be between y_1 and y_2 .

Question 2

November 18, 2020

1 Question 2

For this question I had to replicate the week 7 exercise but using the new ML method for binned data

$$\ln L(v_0, k) = \sum_{i=1}^{N} (n_i ln v_i - v_i)$$

Which was implemented in the third function of the code (L). For the first question it was as simple as implementing the new function like in week 7. To find the uncertainty the graphical method was used like previously.

For part ii I now used scipy.optimize.minimize to minimize the negative function using the Nelder-Mead method. This was used to help with precision problems encountered if you use the default method. Unfortunately I was unable to determine the error this way graphically as I was unsure how to do it used the minimization function.

For part iii I used an uncertainties module (pip install –upgrade uncertainties) to calculate the error propagation on R through the error calculated in part i.

1.1 Final Results

Part i:

$$k = 1.1802 + / -0.0243e - 23\frac{m^2kg}{s^2K}$$

Part ii:

$$k = 1.1804e - 23\frac{m^2kg}{s^2K}$$
$$v_0 = 1.8799e + 03$$

Part iii:

$$N_a = (7.04 + / -0.14)e + 23mol^{-1}$$

1.2 Comments

The results gained are fairly close to the known constants for Boltzmanns constant and Avogadro's number, however they are not within the error bounds which is interesting. For this question you had to pay particular attention to the units. I was unsure how the method was suppose to differ for part ii. I understand you vary both k and v_0 but how to implement this without 2 dimensional

minimization I was unsure. I would also like to know how to determine the uncertainty graphically for part ii. Numerically this is simple but was unsure graphically using scipy.

```
[92]: import numpy as np
      import matplotlib.pyplot as plt
      import scipy.stats
      import scipy.optimize
      from uncertainties import ufloat
      #functions
      def gp_energy(z, r, delta_rho, g): #qravitational potential energy of a_
       \hookrightarrowspherical cluster
          return 4*np.pi * r**3 * delta_rho * g * z / 3
      def poisson(mean_0, z, r, delta_rho, g, k, T): #poisson distribution for random_
       \rightarrow var z
          return v_0 * np.exp(-gp_energy(z, r, delta_rho, g) / (k*T))
      def L(k, mean_0, z, n, r, delta_rho, g, T): #ML binned method
          mean_i = poisson(v_0, z, r, delta_rho, g, k, T)
          return np.sum(n * (np.log(v_0) - gp_energy(z, r, delta_rho, g) / (k*T)) -__
       →mean_i)
      #init
      g = 9.80 #ms/s^2. Says in question 9.80. More accurate result if 9.81 used.
      k const = 1.38064852e-23 # m^2 kg s^2 K s^2 K s^2 True boltzmann constant in Si_{\sqcup}
       \rightarrow units
      r = 0.52e-6 #radius of spheres in meters
      rho_mastic = 1063 \# kg/m^3
      rho_water = 1000 # kg/m^3 approx density of water
      delta_rho = rho_mastic - rho_water
      T = 293 \# K
      focus_thickness = 1e-6 # m
      N bins = 4
      R = 8.314
      #data input
      z = np.array([0, 6, 12, 18])*1e-6 #height, z, in meters
      n = np.array([1880, 940, 530, 305]) #no. clusters
```

```
v_0 = n[0] \#v_0 = n(z=0) = 1880
plt.figure()
plt.bar(z, n, focus_thickness)
plt.ticklabel_format(axis="x", style="sci", scilimits=(0,0))
k_{arr} = np.linspace(1e-24, 1e-22, 10000)
ln_L = np.zeros(10000)
for i in range(k_arr.size):
    ln_L[i] = L(k_arr[i], v_0, z, n, r, delta_rho, g, T)
k_est = k_arr[ln_L_arr.argmax()]
print('All in SI units')
print('----')
print("Actually k:", k_const)
print("Estimated k (Using ML Method for binned data): %1.4e" %k_est)
plt.figure()
plt.plot(k_arr,ln_L)
plt.xlabel('K_arr')
plt.ylabel('ln L')
plt.title('K vs Ln_L')
plt.vlines(k_arr[np.where(ln_L==np.max(ln_L))], 0, 23000, color='green',u
→linestyle='solid')
print('ln L_max = %f' %np.max(ln_L))
print('k = %1.4e (Ordinary ML method)' %k_arr[np.where(ln_L==np.max(ln_L))])
sigma_ln_L = np.max(ln_L) - 0.5
#print('ln L_max_20 - 0.5 = %f' %sigma_ln_L)
k_{unc} = np.linspace(0.1e-22, 0.2e-22, 10000)
ln_L_unc = np.zeros(10000)
for i in range(k_unc.size):
    ln_L_unc[i] = L(k_unc[i], v_0, z, n, r, delta_rho, g, T)
plt.figure()
plt.plot(k_unc,ln_L_unc)
plt.xlabel('f')
plt.ylabel('k_arr')
plt.ylim((22000,22050))
plt.xlim((1.1e-23, 1.3e-23))
plt.title('Parabolic plot centered around the peak at %1.4e' %k_arr[np.
\rightarrowwhere(ln_L==np.max(ln_L))])
plt.hlines(sigma_ln_L, 0.1e-22,0.2e-22, color='red', linestyle='dashed')
idx_f20 = np.argwhere(np.diff(np.sign(ln_L_unc - sigma_ln_L))).flatten()
```

```
#print(idx_f20)
#[1559 2055]
plt.vlines(k unc[1559], 21800, 22030, color='green', linestyle='dashed')
plt.vlines(k_unc[2055], 21800, 22030, color='green', linestyle='dashed')
delta_plus_k = k_arr[np.where(ln_L==np.max(ln_L))] - k_unc[1559]
delta_minus_k = k_unc[2055] - k_arr[np.where(ln_L==np.max(ln_L))]
print('delta +, k= %1.4e' %delta_plus_k) #biggest
print('delta -, k= %1.4e' %delta_minus_k)
print(np.abs(k_est-delta_plus_k),np.abs(k_est-delta_minus_k))
print('\n----')
print('Part (ii):\n')
sol = scipy.optimize.minimize((lambda x, *args: -L(x[0], x[1], *args)),
    x0=np.array([k_est, v_0], dtype=np.longdouble),
    args=(z astype(np.longdouble), n astype(np.longdouble), r, delta_rho, g, T),
    method="Nelder-Mead")
print('k= %1.4e' %sol.x[0])
print('v_0 = \%1.4e' \%sol.x[1])
print('\n----')
print('Part iii:\n')
N_aactual = R / kconst
N_a_{est_i} = R / k_{est_i}
N_a_{est_i} = R / sol.x[0]
w = ufloat(k_est, delta_plus_k)
print('Avogadros number with uncertainty using k from i=', R/w)
print(N_a_est_i)
print('R / k_const = %1.4e' %N_a_actual)
print('Actual N_a = %1.4e' %6.0221409e+23)
All in SI units
Actually k: 1.38064852e-23
Estimated k (Using ML Method for binned data): 1.1802e-23
ln\ L\ max = 22020.138781
k = 1.1802e-23 (Ordinary ML method)
delta +, k = 2.4282e - 25
delta -, k= 2.5323e-25
[1.15591559e-23] [1.15487549e-23]
```

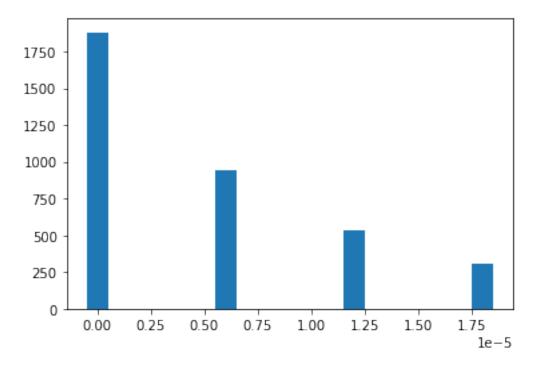
Part (ii):

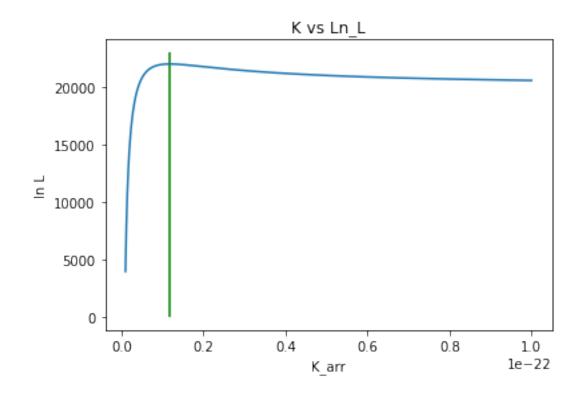
k= 1.1804e-23 v_0 = 1.8799e+03

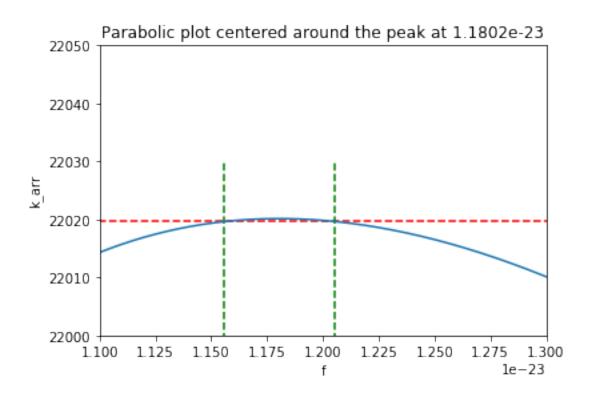
Part iii:

Avogadros number with uncertainty using k from i= (7.04+/-0.14)e+237.044580536912752e+23

 $R / k_const = 6.0218e+23$ Actual $N_a = 6.0221e+23$







```
[69]: #alternative way for part i
      sol = scipy.optimize.minimize((lambda *args: -L(*args)),x0=np.array([k_est],__
      →dtype=np.longdouble),
                                    args=(v_0, z.astype(np.longdouble), n.astype(np.
       →longdouble), r, delta_rho, g, T),
                                    method="Nelder-Mead")
      print(sol)
      final_simplex: (array([[1.18019802e-23],
            [1.18065903e-23]]), array([-22020.13878135, -22020.13874097]))
                fun: -22020.138781348152
            message: 'Optimization terminated successfully.'
               nfev: 16
                nit: 8
             status: 0
            success: True
                  x: array([1.18019802e-23])
 []:
```