final project progession2.0

December 8, 2022

1 Project Description

Since fluorescent proteins have continued to be helpful in new applications of scientific research. Our motivation for this project is that it will help us figure out the matching fluorescents in FRET systemmore efficiently, given a list of fluorescent candidates. For example, scientists can use our code to find the best fluorescent that matches the original fluorescent more efficiently when they discover a new fluorescent protein.

This project aims to use our codes to determine the ideal acceptor fluorescent protein and the donor fluorescent protein. With a given unknown fluorophore in a Förster resonance energy transfer (FRET)system In a FRET system, a donor emits a proton to an acceptor. The wavelength of light the donor emits should fall within the wavelength range that the acceptor can absorb. We will find out the wavelength of the light this unknown protein absorbs and emits. We will match the results with the excitation wavelength range and the emission range with other Fluorescent proteins.

2 Team Member Names and Contributions

2.0.1 Yinuo Song :

Proposed the project topic Develop the main draft Design the functions, loops,and class ### Zhuohao Yuan: Created multiple sets of 1000 points that form a normal distribution with a preset peak value - EGFP emission maximum, mCherry excitation max, and dTomato excitation max; stored these sets into csv files. Created a method that determines which color it is given a peak value by finding the corresponding color in a table, which Yinuo built upon and modified. ### Yining Qi: Prepared CSV data frames of FP protein data with emission and excitation maximum and their corresponding color emission wavelength max and min values. Contributed to partial of the project description.

2.1 Import package

```
[1]: import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
##from absorbancecurve import abso
##from wavelength import wav
##because when the function is called from another notebook file, the numpy is␣
↪always undefined nomatter what
##this notebook will not call function from another notebook
```

2.2 Design 2 functions to generate x,y values for a ditribution curve

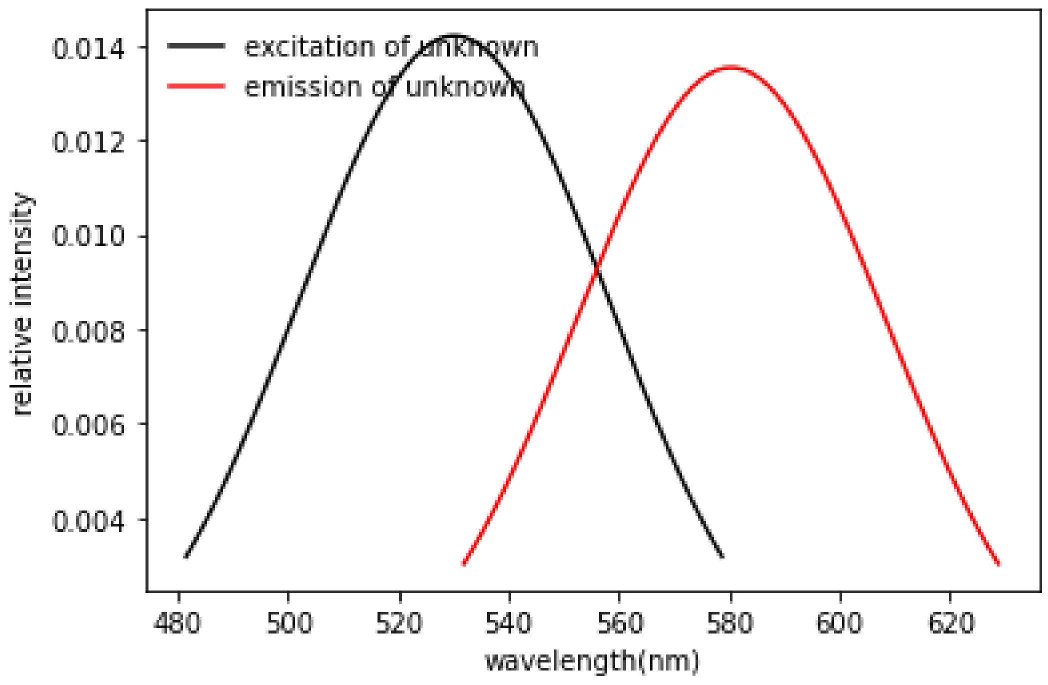
[2]:
```python
##design 2 function that can generate a bell curve with the given data
def abso(x):
    mean=np.mean(x)
    std=np.std(x)
    y= 1/(std * np.sqrt(2 * np.pi)) * np.exp( - (x - mean)**2 / (2 * std**2))
    return y

def wav(x):
    max=np.max(x)
    min=np.min(x)
    y=np.linspace(min,max,1001)
    return y
```

2.3 Read the csv file of lists of the excitation and emission wavelength values of unknown protein into 2 numpy arrays

[21]:
```python
##import the csv files contains the numbers of wavelengths of lights that are␣
↪absorbed or emitted by the unknown protein
##the data is already normalized
##So the mean,median,mode of the data is the same
excitation=np.loadtxt(fname='excitation wavelength.csv', delimiter=',')
emission=np.loadtxt(fname='emission wavelength.csv', delimiter=',')
w1=wav(excitation)
ab1=abso(w1)
w2=wav(emission)
ab2=abso(w2)*0.95
peak_1 = np.mean(excitation)
peak_2 = np.mean(emission)
```

2.4 Create a figure generating the distribution curve

[4]:
```python
##create a figure of the relative intensity of the absorbed light and the␣
↪emitted light
fig, ax = plt.subplots()
plt.plot(w1, ab1, color='black',label='excitation of unknown')
plt.plot(w2, ab2, color='red',label='emission of unknown')
ax.legend(loc='upper left', frameon=False)
plt.xlabel('wavelength(nm)')
plt.ylabel('relative intensity')
plt.show()
```



2.5 Read the color.csv

[5]:
```
##import the color file
df_color = pd.read_csv('color.csv')
df_color.head(7)
```

[5]:
```
    color  wavelength max(nm)  wavelength min(nm)
0     red                 750                 620
1  orange                 620                 590
2  yellow                 590                 570
3   green                 570                 495
4    cyan                 520                 490
5    blue                 495                 450
6  violet                 450                 380
```

2.6 Design a class that has a method to determine color from the wavelength

[6]:
```
##design a class that can determine the color of the light by using the␣
 ↪dataframe above
class Pcolor:
    emc=''
    exc=''
    def __init__(self, exp, emp):
        self.exp = exp
        self.emp = emp
    def findcolor(self):
        for i in range(7):
            if self.exp <df_color.iloc[i,1] and self.exp >df_color.iloc[i,2]:
                self.exc=df_color.iloc[i,0]
                pass
        for i in range(7):
            if self.emp < df_color.iloc[i,1] and self.emp >df_color.iloc[i,2]:
                self.emc=df_color.iloc[i,0]
                pass
```

2.7 Create a object Punknown through Pcolor, imputing the excitation peaks and the emssion peaks

2.8 Find out the color of lights the unknown protein absorbs and emits

[7]:
```
##input the value of the peaks into the new class
##get the color of light
Punknown=Pcolor(peak_1,peak_2)
Punknown.findcolor()
print('The unknown protein absorbs',Punknown.exc,'light.')
print('The unknown protein emits',Punknown.emc,'light.')
```

```
The unknown protein absorbs green light.
The unknown protein emits yellow light.
```

2.9 Read the csv file of the 57 fluorescent proteins

[8]:
```
##import the fluorescent protein file
df_proteinC = pd.read_csv('fluorescent protein.csv')
df_proteinC.head(57)
```

[8]:
```
    Color            Protein  Excitation Maximum(nm)  Emission Maximum (nm)
0    blue               EBFP                     383                    445
1    blue              EBFP2                     383                    448
2    blue            Azurite                     384                    450
3    blue            mTagBFP                     399                    456
4    cyan               ECFP                     439                    476
5    cyan              mECFP                     433                    475
6    cyan           Cerulean                     433                    475
7    cyan              CyPet                     435                    477
8    cyan            AmCyan1                     458                    489
9    cyan   Midori-Ishi Cyan                     472                    495
10   cyan             TagCFP                     458                    480
11   cyan        mTFP1 (Teal)                    462                    492
12  green               EGFP                     484                    507
```

13	green	Emerald	487	509
14	green	Superfolder GFP	485	510
15	green	Azami Green	492	505
16	green	mWasabi	493	509
17	green	TagGFP	482	505
18	green	TurboGFP	482	502
19	green	AcGFP	480	505
20	green	ZsGreen	493	505
21	green	T-Sapphire	399	511
22	yellow	EYFP	514	527
23	yellow	Topaz	514	527
24	yellow	Venus	515	528
25	yellow	mCitrine	516	529
26	yellow	YPet	517	530
27	yellow	TagYFP	508	524
28	yellow	PhiYFP	525	537
29	yellow	ZsYellow1	529	539
30	yellow	mBanana	540	553
31	orange	Kusabira Orange	548	559
32	orange	Kusabira Orange2	551	565
33	orange	mOrange	548	562
34	orange	mOrange2	549	565
35	orange	dTomato	554	581
36	orange	dTomato-Tandem	554	581
37	orange	TagRFP	555	584
38	orange	TagRFP-T	555	584
39	orange	DsRed	558	583
40	orange	DsRed2	563	582
41	orange	DsRed-Express (T1)	555	584
42	orange	DsRed-Monomer	556	586
43	orange	mTangerine	568	585
44	red	mRuby	558	605
45	red	mApple	568	592
46	red	mStrawberry	574	596
47	red	AsRed2	576	592
48	red	mRFP1	584	607
49	red	JRed	584	610
50	red	mCherry	587	610
51	red	HcRed1	588	618
52	red	mRaspberry	598	625
53	red	dKeima-Tandem	440	620
54	red	HcRed-Tandem	590	637
55	red	mPlum	590	649
56	red	AQ143	595	655

2.10 Make the color as index

```
[9]: ##make the color as index
row_index = 'Color'
df_proteinC = df_proteinC.set_index(row_index)
df_proteinC.head()
```

```
[9]:        Protein  Excitation Maximum(nm)  Emission Maximum (nm)
     Color
     blue      EBFP                     383                    445
     blue     EBFP2                     383                    448
     blue   Azurite                     384                    450
     blue   mTagBFP                     399                    456
     cyan      ECFP                     439                    476
```

2.11 Make a new dataframe that contains only green fluorescent protein

```
[10]: (rows,columns)=df_proteinC.shape
##find out protein that emit green light
df_proteinC_emgreen = df_proteinC.loc['green']
df_proteinC_emgreen
```

```
[10]:                Protein  Excitation Maximum(nm)  Emission Maximum (nm)
      Color
      green             EGFP                     484                    507
      green          Emerald                     487                    509
      green  Superfolder GFP                     485                    510
      green      Azami Green                     492                    505
      green          mWasabi                     493                    509
      green           TagGFP                     482                    505
      green         TurboGFP                     482                    502
      green            AcGFP                     480                    505
      green          ZsGreen                     493                    505
      green       T-Sapphire                     399                    511
```

2.12 Make a list of protein names

```
[11]: (grows,gcolumns)=df_proteinC_emgreen.shape
emgreen=[]
for i in range(grows):
    emgreen.append(df_proteinC_emgreen.iloc[i, 0])
emgreen
```

```
[11]: ['EGFP',
       'Emerald',
       'Superfolder GFP',
       'Azami Green',
       'mWasabi',
       'TagGFP',
       'TurboGFP',
       'AcGFP',
       'ZsGreen',
       'T-Sapphire']
```

2.13 Make 'Protein' the index

[12]:
```
##rearrange the index of the dataframe
emgreen_row_index = 'Protein'
df_proteinC_emgreen = df_proteinC_emgreen.set_index(emgreen_row_index)
df_proteinC_emgreen.head()
```

[12]:
```
                  Excitation Maximum(nm)  Emission Maximum (nm)
Protein
EGFP                                 484                    507
Emerald                              487                    509
Superfolder GFP                      485                    510
Azami Green                          492                    505
mWasabi                              493                    509
```

2.14 Define a function that can find the index of fluorescent proteins that absorbs yellow light

[13]:
```
def Excolor(x):
    y=[]
    for i in range(rows):
        if x.iloc[i,1]<df_color.iloc[2,1] and x.iloc[i,1]>df_color.iloc[2,2]:
                y.append(i)
    return y
```

2.15 Find out the row index of proteins that absorb yellow light

[14]:
```
yellow=Excolor(df_proteinC)
##find the row index
print(yellow)
```

```
[46, 47, 48, 49, 50, 51]
```

2.16 Make a dataframe of the proteins that absorb yellow light

[15]:
```
df_proteinC_abyellow = df_proteinC.iloc[46:52]
df_proteinC_abyellow
```

[15]:
```
               Protein  Excitation Maximum(nm)  Emission Maximum (nm)
Color
red        mStrawberry                     574                    596
red             AsRed2                     576                    592
red              mRFP1                     584                    607
red               JRed                     584                    610
red            mCherry                     587                    610
red             HcRed1                     588                    618
```

2.17 Make a list of the names of proteins that absorb yellow light

[16]:
```
##make a list of the names of protein that absorbs yellow light
(yrows,ycolumns)=df_proteinC_abyellow.shape
abyellow=[]
for i in range(yrows):
    abyellow.append(df_proteinC_abyellow.iloc[i, 0])
abyellow
```

[16]:
```
['mStrawberry', 'AsRed2', 'mRFP1', 'JRed', 'mCherry', 'HcRed1']
```

2.18 Make 'Protein' the index

[17]:
```
##rearrange the index of the dataframe
abyellow_row_index = 'Protein'
df_proteinC_abyellow = df_proteinC_abyellow.set_index(abyellow_row_index)
```

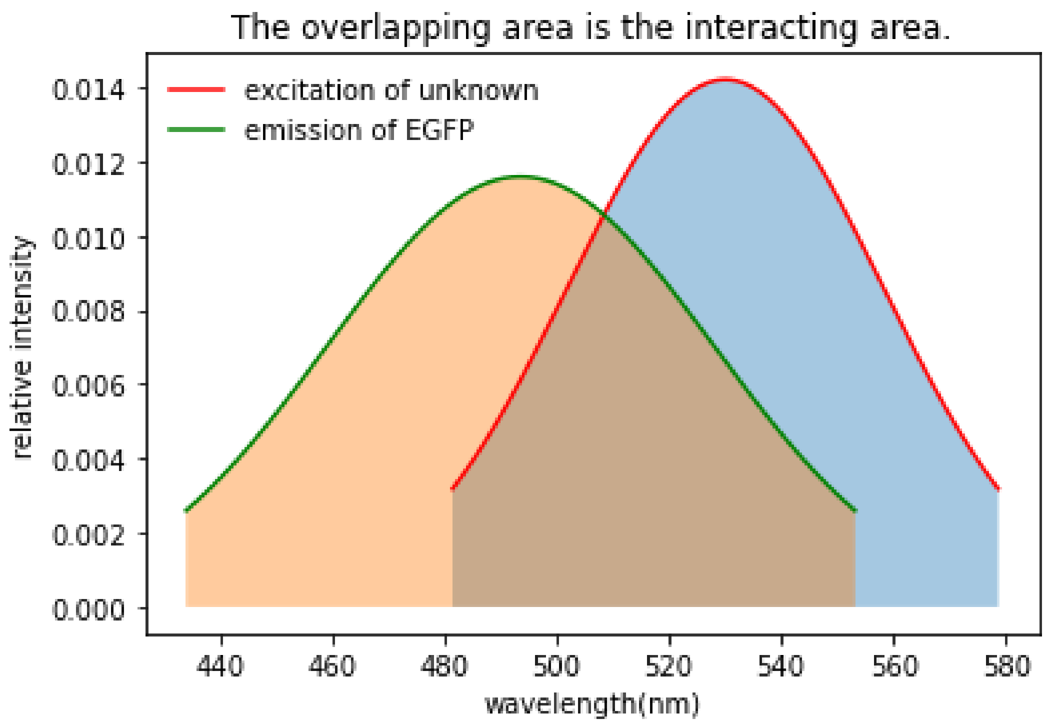
2.19 Print statements of donors and acceptors combination of the unknown protein

[18]:
```
print('The unknown protein can acts as a donor with protein',*abyellow, 'in the␣
↪Förster resonance energy transfer.',sep =',')
print('The unknown protein can acts as an acceptor with protein',*emgreen, 'in␣
↪the Förster resonance energy transfer.',sep =',')
```

```
The unknown protein can acts as a donor with
protein,mStrawberry,AsRed2,mRFP1,JRed,mCherry,HcRed1,in the Förster resonance
energy transfer.
The unknown protein can acts as an acceptor with
protein,EGFP,Emerald,Superfolder GFP,Azami
Green,mWasabi,TagGFP,TurboGFP,AcGFP,ZsGreen,T-Sapphire,in the Förster resonance
energy transfer.
```

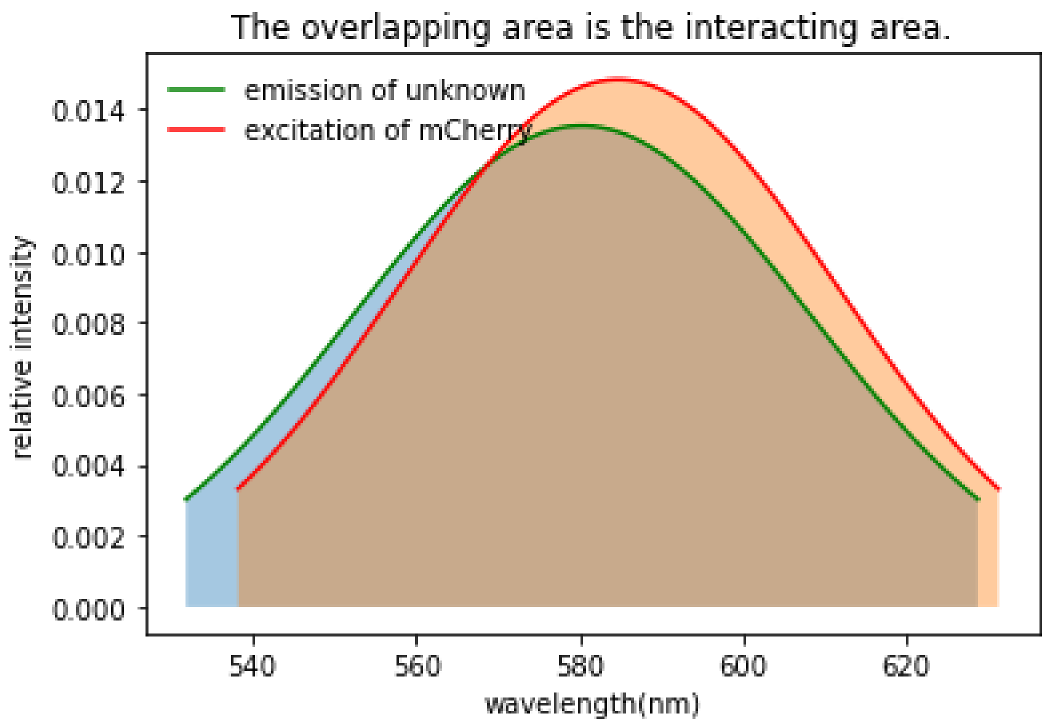
2.20 Import the wavelength csv file of one emgreen protein to check if its emission wavelength range overlaps with the excitation wavelength range of the unknown

[22]:
```
##pick one emgreen protein to make a graph with the unknown protein
EGFP_emission=np.loadtxt(fname='EGFP_emission_max.csv', delimiter=',')
w3=wav(EGFP_emission)
ab3=abso(w3)
fig, ax = plt.subplots()
plt.plot(w1, ab1, color='red',label='excitation of unknown')
plt.plot(w3, ab3, color='green',label='emission of EGFP')
ax.legend(loc='upper left', frameon=False)
plt.title('The overlapping area is the interacting area.')
plt.xlabel('wavelength(nm)')
plt.ylabel('relative intensity')
plt.fill_between(w1, ab1, step="pre", alpha=0.4)
plt.fill_between(w3, ab3, step="pre", alpha=0.4)
plt.show()
```



2.21 Import the wavelength csv file of one abyellow protein to check if its excitation wavelength range overlaps with the emission wavelength range of the unknown

[20]:
```
##pick one abyellow protein to make a graph with the unknown protein
mCherry_excitation=np.loadtxt(fname='mCherry_excitation_max.csv', delimiter=',')
w4=wav(mCherry_excitation)
ab4=abso(w4)
fig, ax = plt.subplots()
plt.plot(w2, ab2, color='green',label='emission of unknown')
plt.plot(w4, ab4, color='red',label='excitation of mCherry')
ax.legend(loc='upper left', frameon=False)
plt.title('The overlapping area is the interacting area.')
plt.xlabel('wavelength(nm)')
plt.ylabel('relative intensity')
plt.fill_between(w2, ab2, step="pre", alpha=0.4)
plt.fill_between(w4, ab4, step="pre", alpha=0.4)
plt.show()
```



3 Reflection

3.0.1 Yinuo Song:

I lead this project. I designed the draft, all the functions and the class. Zhuohao Yuan used codes to generate all the wavelength csv files. Yining Qi generated the fluorescent protein and color csv files from data from Internet. I spend a lot of time on finding how to generate a normal ditribution curve instead of using a histogram. The final method I used is the not the perfect one, but close to what I expected. We had run into problem when generating csv files. When Zhuohao Yuan tried to produce a csv files contains 1000 values using pandas, he generate a file of 1001 with a zero at the beginning. This had caused huge problem for me when using the np.mean and np.min function. We later overcome this problem. When I created the function Excolor, I forgot that Yining has made the color as an index, so the column index number should minus 1. This also cause problems when running the whole notebook. I realize that communcation is really important when coming to groupwork. I had to constantly using a small whiteboard to explain myself. If one notion is stated not clear, my groupmate may get a really weid portion of the code. A lot of time were for debugging and debugging. But we have complete the task perfectly. I like to learn more about python in the future. This experience is really interesting.

3.0.2 Zhuohao Yuan:

I had an awesome time in this class. I had no coding experience before taking this class. I had heard that coding is really hard and debugging can take a long time, and these two factors kept me away from learning how to code. But this course helped me diminish these concerns - as our instructor made concepts really clear and engaging for students to learn. In the assignment where we had to slice a DNA sequence into chunks of three and find out if these chunks match one of two assigned codons, I was challenged because I did not know how to loop through chunks of three - as I only knew we can loop through one item at a time. But after thinking deeply for a while, I found out that I could simply use a list from 1 to 160 (with 480 nucleotides in total) and have it looped through. So I could multiply each item with 3 and then minus 3 and assign this value to be the beginning value of each chunk and assign an item multiplied by 3 as the end value for each codon. And therefore the problem of not being able to loop through chunks of three is solved.

For this final project, it challenged me and expanded my knowledge of coding because as I was creating 1000 values that form a normal distribution. I kept getting a header that shows as zero, which is troubling because once imported, this list becomes 1001 values with the starting value of zero. Therefore, after my research online, I found out that by setting header = None, I could get rid of this zero. This adds to my tool box that I could use further for my future python coding experience. Also, when creating the draft for the method of determining which color it is given a peak value by finding the corresponding color in a table, I could only do a part of the code since I have trouble getting the code to pinpoint the value in the table. My teammate helped me and modified my code to function properly which also expands my knowledge. Therefore, I feel optimistic about coding in the future and working collaboratively with someone else.

3.0.3 Yining Qi:

I came into this class with zero knowledge of Python, Jupiter notebook, and pandas, so I was nervous about practically starting a personal project with the team and doing the task at hand. This class challenged me to think critically about making my code functioning, and I learned a lot more beyond my expectation through referencing class notes and class assignments. I had a great time during this class and a good experience working with my final project team. The group project challenged me to think creatively and be exposed to the field of fluorescent proteins, which was new for me. As a freshman in the project topics, this final project reminds me of the growth I have experienced by looking for protein data with their corresponding colors and getting to know their application. Besides that, as a new coder, being able to use pandas to manipulate CSV data frames amazed me. Some aspects of the project were challenging, but overall, with teamworks and researching the topics; it was a fun expereince.