

```
In [1]: import numpy as np
from scipy.integrate import odeint
from scipy.optimize import curve_fit
from scipy.optimize import differential_evolution
%matplotlib inline
import matplotlib.pyplot as plt
from matplotlib.backends.backend_pdf import PdfPages
import pandas as pd
```

```
In [2]: from endpoint_maker import sqres
from endpoint_maker import func
from endpoint_maker import t
from endpoint_maker import new
from endpoint_maker import lightdata
from endpoint_maker import rawdata
```

```
In [3]: if __name__ == '__main__':
def initparams():
    #bounds = ([0.00001,10000],[0,4],[0.00001,1000],[0.00001,1000],[0.00001,10000])
    bounds = ([0.00001,1000],[0.00001,1000],[0.00001,10000],[0.00001,10000])
    result = differential_evolution(sqres,bounds,maxiter=100,popsize=20,polipopsize=20)
    return result
```

```
In [4]: initialp = initparams()
print(initialp)
```

```
message: Maximum number of iterations has been exceeded.
success: False
  fun: 0.2772146402881579
   x: [ 3.715e+02  1.514e-03  1.468e-04  9.449e+03]
  nit: 100
 nfev: 8080
```



```

In [5]: #def tester(t,Kd,n,d2,k2,k3,i):
def tester(t,d2,k2,k3,k7,i):

    inivalues = [1,0,0,0,0,0,0]
    arrayvalues = np.asarray([])

    #for i in range(len(Lightdata[:,0])):
    def I(t):
        tindex = t/5
        if tindex > 12241:
            tindex = 12240
        return lightdata[i][int(tindex)]

    #def odes(z,t,Kd,n,d2,k2,k3):
    def odes(z,t,d2,k2,k3,k7):
        Pu,Pb,Pa,mRNA,mCherry1,mCherry2,mCherry3 = z
        d1 = 0.019905
        k1 = 0.08299
        Kd = 90.41
        n = 0.964487
        #d2= 486.67
        #k2= 6.597
        #k3= 0.0539

        d3 = 0.000077
        k4 = 1.25
        d4 = 0.000031
        k5 = 0.00283
        k6 = 0.00283

        Pu = z[0]
        Pb = z[1]
        Pa = z[2]
        mRNA = z[3]
        mCherry1 = z[4]
        mCherry2 = z[5]
        mCherry3 = z[6]

        dPudt = d1*Pb - k1*I(t)*Pu - k7*I(t)**n/(Kd**n+I(t)**n)*Pu
        dPbdt = k1*I(t)*Pu - k2*Pb - d1*Pb + d2*Pa
        dPadt = k2*Pb - d2*Pa + k7*I(t)**n/(Kd**n+I(t)**n)*Pu
        dmRNAAdt = k3*Pa - d3*mRNA
        dmCherry1dt = k4*mRNA-(d4 + k5)*mCherry1
        dmCherry2dt = k5*mCherry1-(d4+k6)*mCherry2
        dmCherry3dt = k6*mCherry2 - d4*mCherry3

        return [dPudt,dPbdt,dPadt,dmRNAAdt,dmCherry1dt,dmCherry2dt,dmCherry3dt]

    #solver = odeint(odes,inivalues,t,args = (Kd,n,d2,k2,k3),hmax=0.1)
    solver = odeint(odes,inivalues,t,args = (d2,k2,k3,k7),hmax=0.1)

    mCherryout = solver[:,6]
    #mCherryout = mCherryout[0:24480:240]

```

```
return mCherryout
```

In [6]: `print(initialp.x)`

```
[3.71500918e+02 1.51356699e-03 1.46768590e-04 9.44871064e+03]
```

In [7]: `popt, covt = curve_fit(func,t,new,initialp.x,maxfev=1000000)`

```
#popt, covt = curve_fit(func,t,newdata,initialp.x, maxfev=10000000, bounds=((0
#popt, covt = curve_fit(func,t,newdata,initialp.x, maxfev=1000000)
```

```
#Kd,n,d2,k2,k3 = pop
#print('Kd=',Kd,'n=',n,'d2=',d2,'k2=',k2,'k3=',k3)
```

```
#d3,k4,d4,k5,k6 = pop
#print('d3=',d3,'k4=',k4,'d4=',d4,'k5=',k5,'k6=',k6)
```

```
d2,k2,k3,k7 = pop
print('d2=',d2,'k2=',k2,'k3=',k3,'k7=',k7)
```

C:\Users\Leandra\anaconda3\Lib\site-packages\scipy\integrate_odepack_py.py:248: ODEintWarning: Excess work done on this call (perhaps wrong Dfun type). Run with full_output = 1 to get quantitative information.

warnings.warn(warning_msg, ODEintWarning)

```
d2= 372.50603793656074 k2= 0.0015605798854391216 k3= 0.00014692733294994307 k
7= 13317.448906558491
```

```
In [8]: import sys
import numpy
#params = [1,1,1,1,1,1,1]
params = [1,1,1,1]
numpy.set_printoptions(threshold=10)
#model1 = np.asarray(func(t,Kd,n,d2,k2,k3))
model1 = np.asarray(func(t,d2,k2,k3,k7))
print(len(model1))
#print(model1)

#a,b,c,d,e,f,g = params
a,b,c,d = params

ydata = np.asarray(new)
print(len(ydata))

ssr = np.sum((ydata-model1)**2)
#ssr2 = np.sum((ydata-model2)**2)
sst = np.sum((ydata - np.mean(ydata))**2)
R2 = 1 - ssr/sst
#R2_2 = 1 - ssr2/sst

print('R2 is: ', R2)
#print(R2_2)
```

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R2 is: 0.8425766248609146

```

In [9]: pp = PdfPages('multipage.pdf')
        ydata = np.asarray(new)

        #condition = [1,2,3,4,5,6,7,8,9]
        for i in range(2):
            #model = tester(t,Kd,n,d2,k2,k3,i)
            model = tester(t,d2,k2,k3,k7,i)

            #print(model)
            #a,b,c,d,e,f,g= params
            a,b,c,d= params

            plt.plot(t,model,'.', label = 'model')
            #print(model)
            #t = np.linspace(0,34800, num=6961)
            #raw = rawdata[0:13920:240]
            plt.plot(t,raw[i],'.',label = 'data')
            #print(rawdata[i])
            plt.legend()
            pp.savefig()
            plt.show()

pp.close

```

NameError

Traceback (most recent call last)

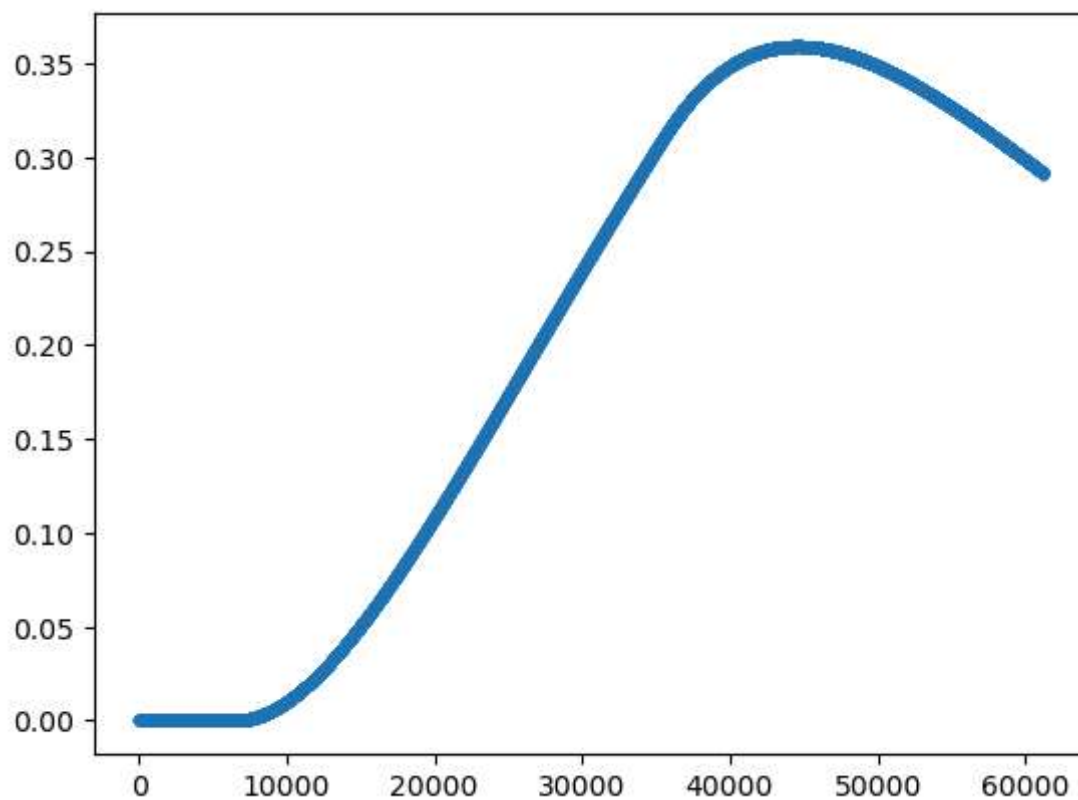
Cell In[9], line 17

```

13 plt.plot(t,model,'.', label = 'model')
14 #print(model)
15 #t = np.linspace(0,34800, num=6961)
16 #raw = rawdata[0:13920:240]
---> 17 plt.plot(t,raw[i],'.',label = 'data')
18 #print(rawdata[i])
19 plt.legend()

```

NameError: name 'raw' is not defined



In []: