

```
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],[0.00001,100
    bounds = ([0.001,10],[0.001,10],[0.001,10],[0.001,10])
    result = differential_evolution(sqres,bounds,maxiter=500,popsize=20,polish=
    return result
```

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

```
message: Optimization terminated successfully.
success: True
  fun: 5.81059447153127
    x: [ 9.998e+00  1.000e-03  1.000e-03  9.593e+00]
  nit: 107
 nfev: 8640
```

```
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[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)**n/(Kd**n+I(t)**n)*Pu + k7*I(t)*Pa
dPbdt = k1*I(t)**n/(Kd**n+I(t)**n)*Pu - k2*Pb - d1*Pb + d2*Pa
dPadt = k2*Pb - d2*Pa - k7*I(t)*Pa
dmRNA dt = 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,dmRNA dt, 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)`

```
[9.99836644e+00 1.00021253e-03 1.00001552e-03 9.59250908e+00]
```

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=((0.0000
#popt, covt = curve_fit(func,t,newdata,initialp.x, maxfev=1000000)

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

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

d2,k2,k3,k7 = popl
print('d2=',d2,'k2=',k2,'k3=',k3,'k7=',k7)

```

```
C:\Users\Leandra\endpoint-fitter\endpoint_maker.py:58: RuntimeWarning: invalid value
encountered in scalar multiply
    dPudt = d1*Pb - k1*I(t)**n/(Kd**n+I(t)**n)*Pu + k7*I(t)*Pa
C:\Users\Leandra\endpoint-fitter\endpoint_maker.py:60: RuntimeWarning: invalid value
encountered in scalar multiply
    dPadt = k2*Pb - d2*Pa - k7*I(t)*Pa
C:\Users\Leandra\anaconda3\Lib\site-packages\scipy\integrate\_odepack_py.py:248: ODE
intWarning: Excess accuracy requested (tolerances too small). Run with full_output =
1 to get quantitative information.
    warnings.warn(warning_msg, ODEintWarning)
d2= 12.525429814300974 k2= 0.0007386970054642127 k3= 0.00045012038491597613 k7= 6.43
5509464527216
```

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

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R2 is: 0.8224517142216978

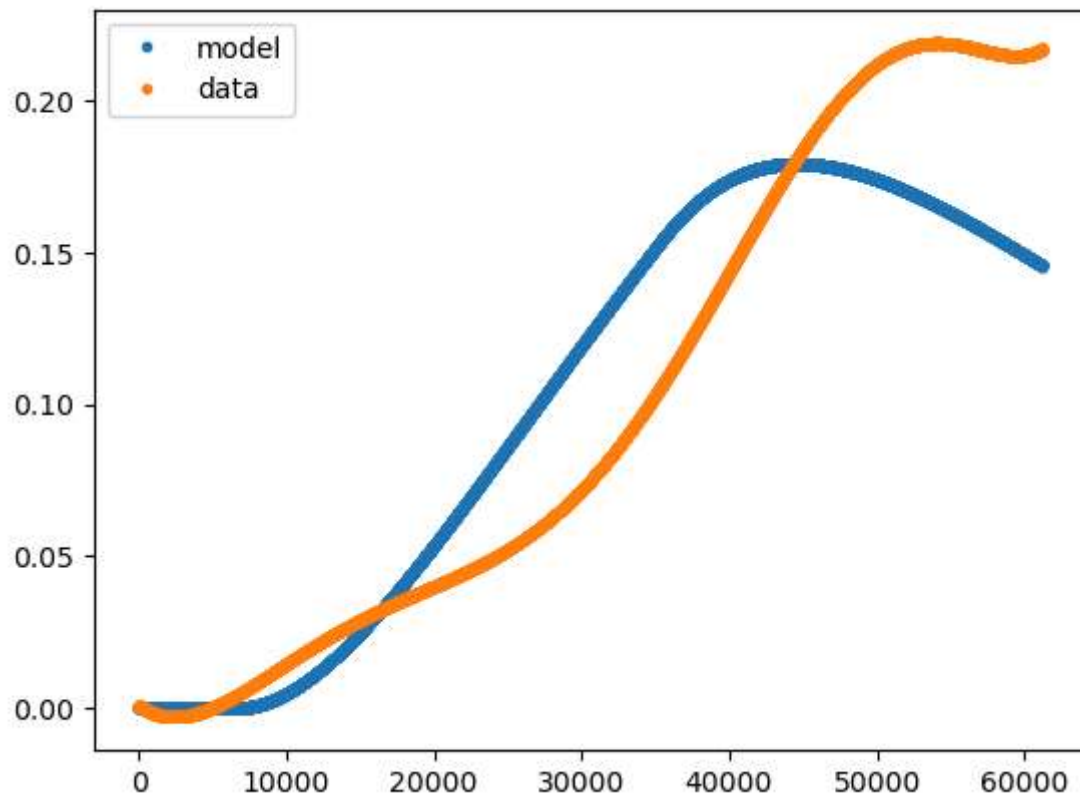
```
In [9]: pp = PdfPages('multipage.pdf')
ydata = np.asarray(new)

#condition = [1,2,3,4,5,6,7,8,9]
for i in range(1):
    #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,rawdata,'.',label = 'data')
```

```
#print(rawdata[i])  
plt.legend()  
pp.savefig()  
plt.show()  
  
pp.close
```



Out[9]: <bound method PdfPages.close of <matplotlib.backends.backend_pdf.PdfPages object at 0x000001D089AB3ED0>>

In []:

In []: