

Answer to question 2

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Question 2: Enzyme Kinetics

2.1

By the Law of Mass Action:

$$\frac{dE}{dt} = (ES) \cdot (k_2 + k_3) - E \cdot S \cdot k_1 \quad (1)$$

$$\frac{dS}{dt} = (ES) \cdot k_2 - E \cdot S \cdot k_1 \quad (2)$$

$$\frac{d(ES)}{dt} = (ES) \cdot k_1 - (ES) \cdot (k_2 + k_3) \quad (3)$$

$$\frac{dP}{dt} = (ES) \cdot k_3 \quad (4)$$

2.2

Assumptions from the question:

The initial concentration $E_0 = 1\mu M$, $S_0 = 10\mu M$, $(ES)_0$ and P_0 are both 0.
 $k_1 = 100\mu M/min$, $k_2 = 600\mu M/min$, $k_3 = 150\mu M/min$.

The four equations above,

```
# y = c(ES, E, S, P)
f1 <- function(t, y) {
  out <- c(0, 0, 0, 0)
  out[1] = 750*y[1] - 100*(y[2]*y[3]) # equation (1)
  out[2] = 600*y[1] - 100*(y[2]*y[3]) # equation (2)
  out[3] = 650*y[1] # equation (3)
  out[4] = 150*y[1] # equation (4)
  return(out)
}
```

The fourth-order Runge-Kutta method

```

runge_kutta4 <- function(a,b,f,y0,N) {
#Parameters
# a,b: start and end of the interval
# f: The function to be solved using RK4
# y0: The initial conditions c(E0,S0,ES0,P0)
# N: Number of time-steps to take

#Returns
#t: representing the points at which the function is approximated
#y: contains the approximations to f given initial condition y0

t = c(rep(0,N))
y = matrix(c(rep(0,4*N)),nrow = 4,ncol = N)

h = (b-a)/N # Step size h

t[1] = a
t0 = t[1]
y[,1] = y0
# Initial condition

for (i in 2:N){
  t[i] = a +i*h
  k1 <- f(t0,y0)
  k2 <- f(t0+h/2, y0+(h/2)*k1)
  k3 <- f(t0+h/2, y0+(h/2)*k2)
  k4 <- f(t0+h/2, y0+h*k3)
  y[,i] = y0 + (h/6)*(k1+2*k2+2*k3+k4) # Set up for the 4th order RK method.
  y0 = y[,i]
  t0 = t[i]
}

return(list(time = t,values = y)) # return the time points and approximated values
}

```

call the function

```

y0 <- c(1,10,0,0)
out1 <- runge_kutta4(0,0.001,f1,y0,5)
print(out1$time) #time points

```

```
## [1] 0e+00 4e-04 6e-04 8e-04 1e-03
```

```
print(out1$values) #approximate values at each time points
```

```
##      [,1]      [,2]      [,3]      [,4]      [,5]
## [1,]    1  1.14737823  1.28580244  1.4092774  1.5114049
## [2,]   10 10.11515209 10.21704882 10.3000523 10.3583079
## [3,]    0  0.13964663  0.29793234  0.4733090  0.6634203
## [4,]    0  0.03222614  0.06875362  0.1092252  0.1530970
```

Comments: The results show approximated values of the four equations in 2.1. The choice of the time interval is from 0 to 0.001 minutes. When choosing a bigger time interval, the concentration is increasing very fast to a high amount and making it difficult to observe the change from initial conditions. This might be because the enzyme has a significant catalytic effect on the reaction, so the concentration might change significantly in a short period.

However, the results seem unconvincing since, all four species, E, S, ES, and P are increasing. There should be a reduction for some species during the reaction process due to the negative/positive feedback systems, although the enzymes are not changed by the reaction. Thus, there might be some problems in 2.1 where the four equations are wrong, or there might be some problems in the code for the fourth-order Runge Kutta method.

2.3

By $\frac{dP}{dt} = (ES) \cdot k_3$ (4) in 2.1, we need to express (ES) using S.

Since the enzymes are not changed by the reaction. We get:

$$E_{free} + ES = E_0,$$

thus,

$$k_1(E_0 - ES)(S) = (k_2 + k_3)(ES)$$

rearrange,

$$ES = \frac{(E_0)(S)}{S + \frac{k_2+k_3}{k_1}} \quad (5)$$

therefore, by (4) and (5)

$$V = \frac{dP}{dt} = \frac{k_3(E_0)(S)}{S + \frac{k_2+k_3}{k_1}} \quad (6)$$

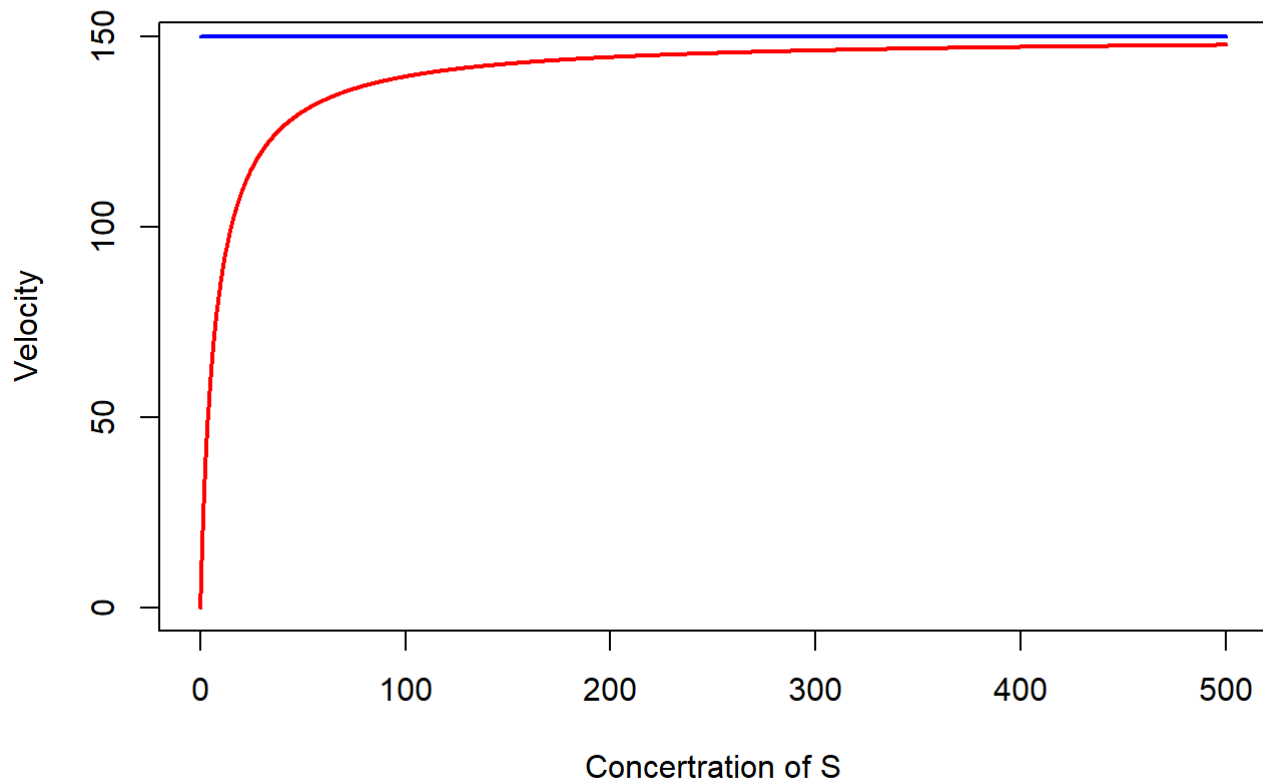
Substitute k_1, k_2, k_3 into (6),

$$V = \frac{150S}{S + 7.5} \quad (7)$$

Plot V against S,

```
S <- seq(0, 500, by = 0.1)
V = 150*S/(S+7.5)
plot(S,V,type="l", lwd=2, col="red", main = "Plot V as a function of the concentration of S", xlab = "Concentration of S", ylab = "Velocity")
lines(S,S*0+150,lwd=2, col="blue")
```

Plot V as a function of the concentration of S



From (7), we know that when S is small, the function is approximately linear, since the denominator is $7.5 + S$, S in the denominator is negligible when S is small. We can see V_m is 150 from the plot.