Q2 codes - Zhiqi Tang

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set initial conditions

```
E0=1
S0=10
ES0=0
P0=0
vars0<-c(E0, S0, ES0, P0)
```

set parameters

```
k1=100/60
k2=600/60
k3=150/60
parms<-c(k1, k2, k3)
```

set time sequence (solve for 50 secs, 1 sec per timestep)

```
end.time<-50
time.seq<-seq(0,end.time,1)
```

define function

```
Enzyme.model <- function(t, vars, parms){
  E<-vars[1]
  S<-vars[2]
  ES<-vars[3]
  P<-vars[4]

  k1<-parms[1]
  k2<-parms[2]
  k3<-parms[3]
```

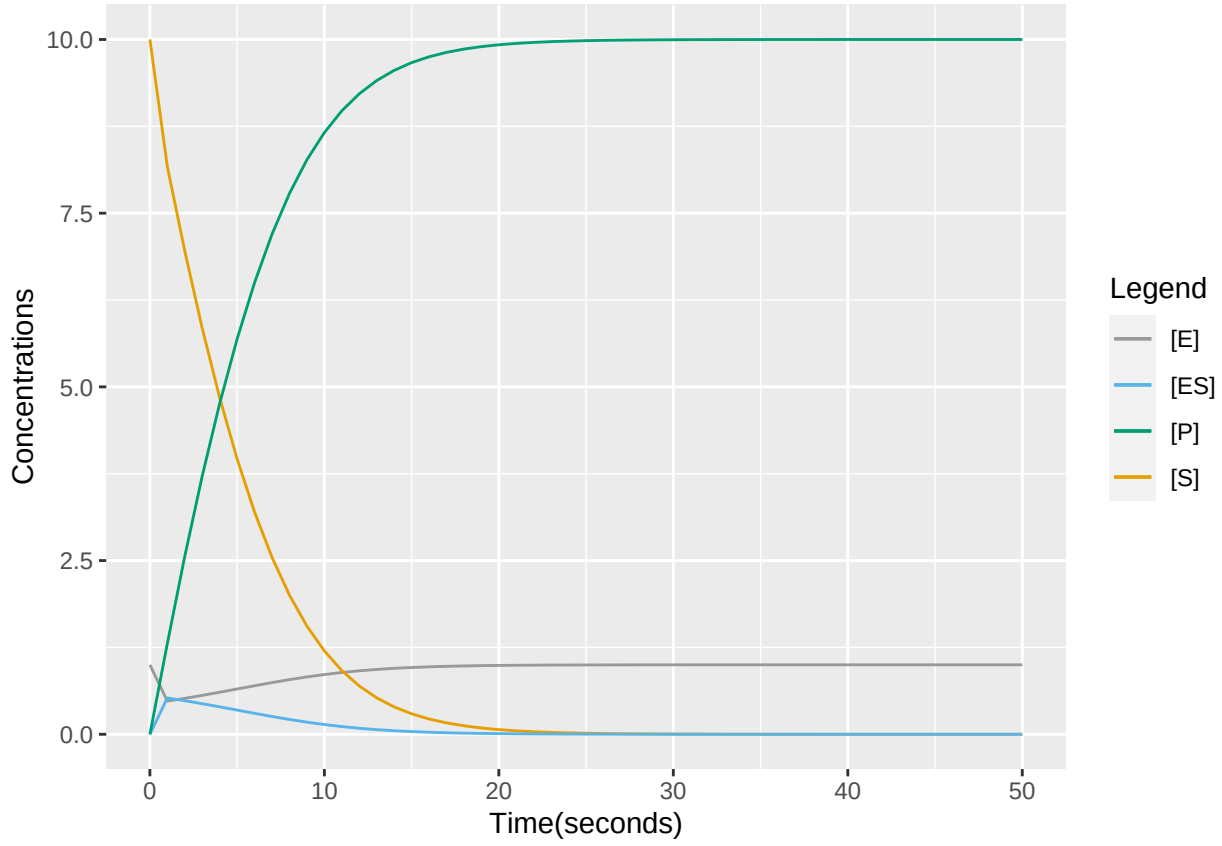
```
  dE = k2*ES + k3*ES - k1*E*S
  dS = k2*ES - k1*E*S
  dES = k1*E*S - k2*ES - k3*ES
  dP = k3*ES

  return(list(c(dE, dS, dES, dP)))
}
```

store results in dataframe

```
Enzyme.output1<-lsoda(vars0, time.seq, Enzyme.model, parms)
colnames(Enzyme.output1)[2:5]<-c("E", "S", "ES", "P")
Enzyme.output1<-as.data.frame(Enzyme.output1)
```

plot results in graph

```
colors <- c("[E]"="#999999", "[S]"="#E69F00", "[ES]"="#56B4E9", "[P]"="#009E73")

ggplot(data=Enzyme.output1,aes(x=time))+geom_line(aes(y=E,color="[E]"))+geom_line(aes(y=S,color="[S]"))+
```



set new initial conditions

```
delta0=0
newvars0<-c(E0, S0, ES0, P0, delta0)
```

define function

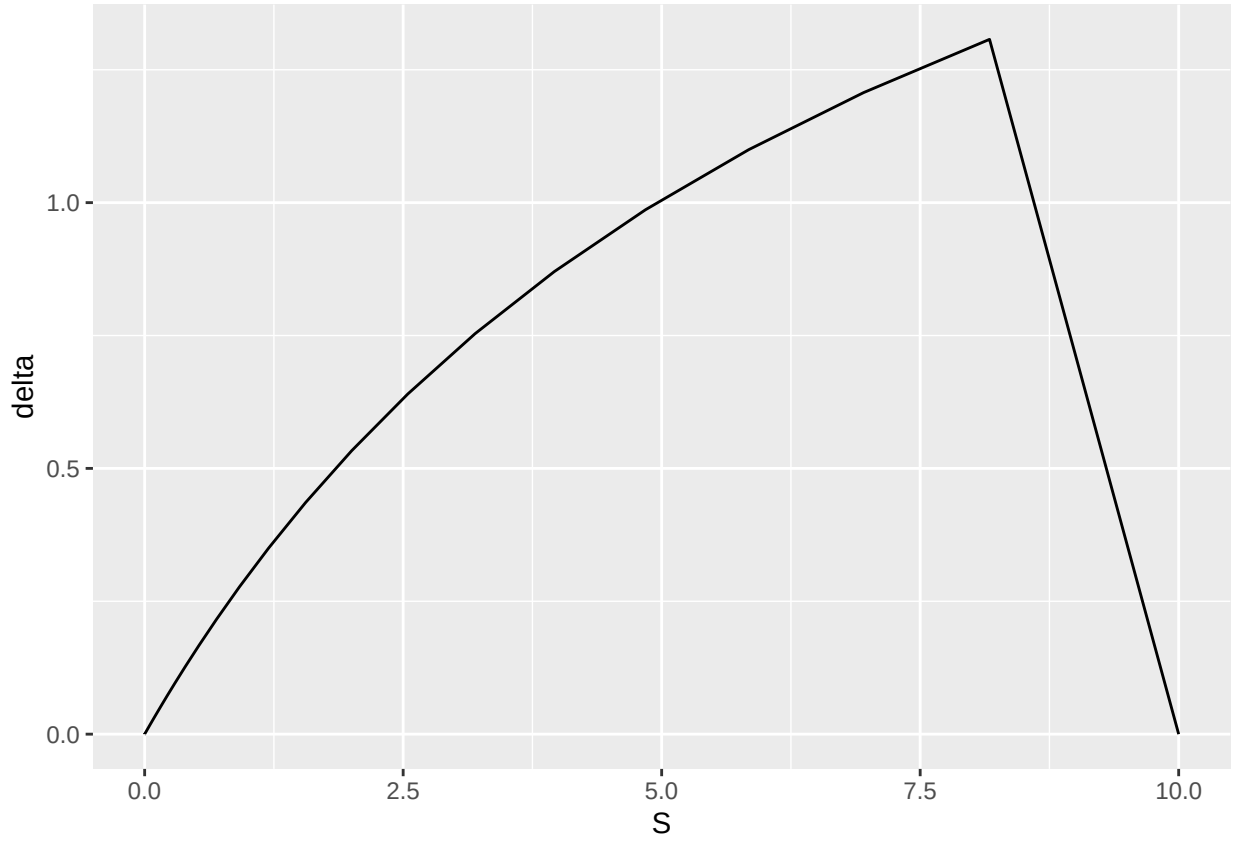
```
V.model <- function(t, vars, parms){
  E<-vars[1]
  S<-vars[2]
  ES<-vars[3]
  P<-vars[4]
  delta<-vars[5]

  k1<-parms[1]
  k2<-parms[2]
  k3<-parms[3]

  dE = k2*ES + k3*ES - k1*E*S
  dS = k2*ES - k1*E*S
  dES = k1*E*S - k2*ES - k3*ES
  dP = k3*ES
  delta = k3*(k1*E*S - k2*ES - k3*ES)
  #note that d(dp/dt)/dt = k3*dES/dt

  return(list(c(dE, dS, dES, dP, delta)))
}
```

store results in dataframe

```
V.output1<-lsoda(newvars0, time.seq, V.model, parms)
colnames(V.output1)[2:6]<-c("E", "S", "ES", "P", "delta")
V.output1<-as.data.frame(V.output1)
```

plot V against S

```
ggplot(data = V.output1)+geom_line(aes(x=S,y=delta))
```



the plot shows Vm ~ 1.307 at S0 = 10.