Homework 4 (Part 1)

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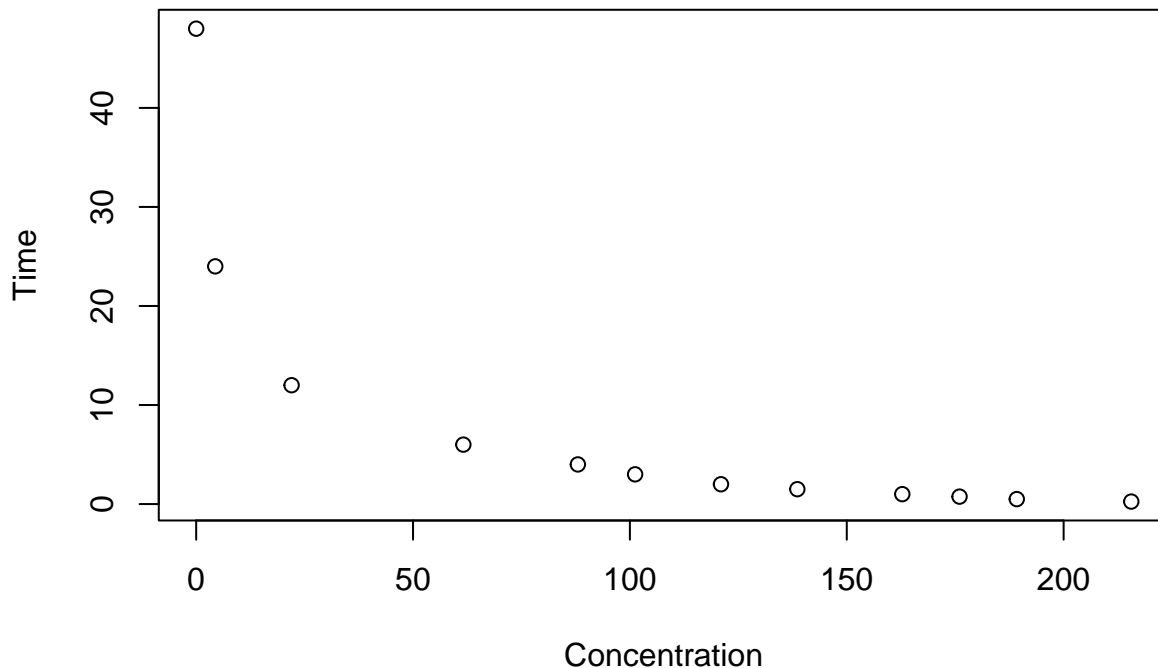
Part (a).

```r
### using the R functino nls() to apply GAUSSNEWTON algorithm solution. Make trace=T to show the iterat

# data importation
df <- read.table("serum_conc.txt", head = T)
attach(df)

# build model
model <- function(t,a1,a2,l1,l2){
  E_1 = exp(-l1*t)
  E_2 = exp(-l2*t)
  f = a1*E_1 + a2*E_2
  grad = cbind(E_1,E_2,-a1*t*E_1, -a2*t*E_2)
  attr(f,'gradient') <- grad
  f
}

# nls fit
plot(Concentration,Time)
```

```r
nls_fit <-  nls(Concentration ~ model(Time,a1,a2,l1,l2),
                start = list(a1=100,a2=100,l1=0.05,l2=0.1),
                trace = T,
                nls.control(maxiter = 50, tol = 1e-5, minFactor = 1/1024,
                            printEval=TRUE))
```

```
## Warning in min(x): no non-missing arguments to min; returning Inf

## Warning in max(x): no non-missing arguments to max; returning -Inf

## 22333.66    (4.93e+00): par = (100 100 0.05 0.1)
## 22208.92    (5.23e+00): par = (128.775 71.35681 0.05465001 0.1143425)
## 22038.24    (5.56e+00): par = (146.7226 53.56492 0.05735114 0.1313065)
## 21879.61    (6.29e+00): par = (166.2577 34.38963 0.06067186 0.1683894)
## 20834.84    (7.66e+00): par = (178.1465 23.40306 0.06413547 0.2552384)
## 16473.59    (9.47e+00): par = (175.8112 28.14394 0.06790986 0.4345737)
## 9151.242    (9.26e+00): par = (162.9695 47.24893 0.07469691 0.6479215)
## 2538.979    (6.39e+00): par = (146.31 76.43212 0.09068339 0.8208273)
## 117.5745    (1.56e+00): par = (143.0741 96.10459 0.1295516 1.018437)
## 39.94938    (4.08e-01): par = (160.9446 82.02848 0.1594032 1.21782)
## 34.46871    (5.10e-02): par = (163.1019 80.84257 0.1622768 1.313193)
## 34.38037    (1.92e-03): par = (162.5701 81.25335 0.1617604 1.305126)
## 34.38026    (2.17e-04): par = (162.6015 81.23977 0.1617944 1.306174)
## 34.38026    (2.52e-05): par = (162.5976 81.24147 0.1617903 1.306053)
## 34.38026    (2.93e-06): par = (162.598 81.24128 0.1617907 1.306067)
```

```r
summary(nls_fit)
```

```
##
## Formula: Concentration ~ model(Time, a1, a2, l1, l2)
##
## Parameters:
##     Estimate Std. Error t value Pr(>|t|)
## a1 162.59804    6.94317  23.418 1.18e-08 ***
```

```
## a2  81.24128     6.10752  13.302 9.74e-07 ***
## l1   0.16179     0.00878  18.427 7.75e-08 ***
## l2   1.30607     0.19757   6.611 0.000168 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 2.073 on 8 degrees of freedom
##
## Number of iterations to convergence: 14
## Achieved convergence tolerance: 2.928e-06
```

Part (b).

```
plot(Time, Concentration)
t = seq(0,50,.1)
lines(t,162.5980*exp(-0.1618*t)+81.2413*exp(-1.3061*t), col = 'blue')
# Mori's line
lines(t,211.9203*exp(-0.2357*t),col='red')
```