

1. Use biochemical oxygen demand (BOD) data set.

- (a) Possible values are:  $b_1^0 = 225$ ,  $b_2^0 = 0.67$ .
- (b) 

```
BOD.fm <- nls(formula=y~b1*(1-exp(-b2*x)),start=c(b1=225,b2=0.67),trace=T)
> BOD.fm
Nonlinear regression model
model: y ~ b1 * (1 - exp(-b2 * x))
data: parent.frame
      b1      b2
213.8092235  0.5472396
residual sum-of-squares: 1168.009
```
- (c) 

```
time <- seq(0,11,0.1)
biochemical <- coef(BOD.fm)[1]*(1-exp(-coef(BOD.fm)[2]*time))
plot(c(0,11),c(0,250),type="n",xlab="Time (min)",ylab="BOD (mg/l)")
points(x,y)
lines(time,biochemical)
```
- (d) 

```
> summary(BOD.fm)
Formula: y ~ b1 * (1 - exp(-b2 * x))

Parameters:
  Estimate Std. Error t value Pr(>|t|)
b1 213.8092    12.3545  17.306 6.54e-05 ***
b2  0.5472     0.1046   5.234 0.00637 **
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 17.09 on 4 degrees of freedom

Correlation of Parameter Estimates:
      b1
b2 -0.7298

> vcov(BOD.fm)
      b1      b2
b1 152.6333128 -0.94280584
b2 -0.9428058  0.01093288
 $f(x, b) = b_1(1 - \exp(-b_2x))$ .  $\hat{D} = (1 - \exp(-b_2x)|_{b_2=0.5472}, b_1 x \exp(-b_2x)|_{b_1=213.8092, b_2=0.5472})$ .
```
- ```
b1 <- coef(BOD.fm)[1] ; b2 <- coef(BOD.fm)[2]
Dhat <- matrix(c(1-exp(-b2*x),b1*x*exp(-b2*x)),6,2)
> deviance(BOD.fm)/4*solve(t(Dhat)%*%Dhat)
      [,1]      [,2]
[1,] 152.6333112 -0.94280581
[2,] -0.9428058  0.01093288
```
- (e)  $\hat{x} = -\frac{1}{0.5472} \log(1 - \frac{100}{213.8092}) = 1.15$ . Let  $h(b_1, b_2) = -\frac{1}{b_2} \log(1 - \frac{100}{b_1})$ .  
Then  $\hat{G} = \left( -\frac{1}{b_2} \frac{100/b_1^2}{1-100/b_1} \Big|_{b_{OLS}}, \frac{1}{b_2^2} \log(1 - \frac{100}{b_1}) \Big|_{b_{OLS}} \right)$ .
- ```
xhat <- -(1/b2)*log(1-100/b1)
Ghat <- matrix(c((-1/b2)*(100/b1^2)/(1-100/b1), (1/b2^2)*log(1-100/b1)),1,2)
> sqrt(Ghat%*%vcov(BOD.fm)%*%t(Ghat))
[1,] 0.1651142
```

```
(f) ss <- function(b1,b2) {
  tmp <- 0
  for (i in 1:length(y)) tmp <- tmp + (y[i]-b1*(1-exp(-b2*x[i])))^2
  tmp
}
beta1 <- seq(150,300,1)
beta2 <- seq(.2,1.4,.01)
SumofSquares <- outer(beta1,beta2,FUN=ss)
contour(beta1,beta2,SumofSquares,levels=seq(1000,10000,500))
```

To obtain the Beale 90% confidence region for the parameter vector  $(\beta_1, \beta_2)$ , we need to consider the pairs  $(\beta_1, \beta_2)$  with sum of squares less than 3694.

```
> ss(b1,b2)*(1+(2/4)*qf(0.90,2,4))
3693.568
```

This region suggests a wide range of possible values of  $\beta_1$  (visually between 175 and 260). This indicates that the data does not allow to identify the limiting BOD with much precision.

(g) Consider the values of  $\beta_1$  for which there is a  $\beta_2$  with sum of squares less than 2495. Visually the interval for  $\beta_1$  is (185, 245).

```
> ss(b1,b2)*(1+(1/4)*qf(0.90,1,4))
2495.092
```

(h) The interval for  $\beta_1$  (187, 240) is similar to the one obtained in (g).

```
ll <- b1 - qt(0.95,4)*sqrt(vcov(BOD.fm)[1])
ul <- b1 + qt(0.95,4)*sqrt(vcov(BOD.fm)[1])
```