HW 1 Solutions

1) As derived in class, the likelihood function is:

$$f(y_1, y_2, \ldots, y_n; \mu, \sigma) = \frac{1}{(2\pi)^{n/2}\sigma^n} exp\left\{-\frac{1}{2\sigma^2}\sum_{i=1}^{n}(y_i-\mu)^2\right\}$$

Setting the partial derivative with respect to σ equal to zero gives:

$$\frac{\partial f(y_1, y_2, \cdots y_n; \mu, \sigma)}{\partial \sigma} = \frac{1}{(2\pi)^{n/2}\sigma^n} exp\left\{-\frac{1}{2\sigma^2}\sum_{i=1}^{n}(y_i-\mu)^2\right\}\frac{1}{\sigma^3}\sum_{i=1}^{n}(y_i-\mu)^2 - \frac{n}{(2\pi)^{n/2}\sigma^{n+1}} exp\left\{-\frac{1}{2\sigma^2}\sum_{i=1}^{n}(y_i-\mu)^2\right\} = 0$$

Canceling out common factors gives

$$\frac{1}{\sigma^3}\sum_{i=1}^{n}(y_i-\mu)^2 - \frac{n}{\sigma} = 0 .$$

Solving for σ and plugging in the MLE for μ ($\hat{\mu} = \bar{y}$) gives

$$\hat{\sigma} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i-\bar{y})^2} .$$

2) The linear regression approach in part (a) gives starting values $\hat{\gamma}_0$ = 29.6 and $\hat{\gamma}_1$ = 13.4. The nlm() script and output is (including results we will use for the next problem):

```
> Enz<-read.table("Enz.csv",sep=",",header=TRUE)
> x=Enz$x
> y=Enz$y
> out<-nlm(function(p) sum((y-p[1]*x/(p[2]+x))^2),p=c(29.6,13.4),hessian=TRUE)
> theta<-out$estimate  #parameter estimates
> MSE<-out$minimum/(length(y) - length(theta))  #estimate of the error variance
> InfoMat<-out$hessian/2/MSE  #observed information matrix
> CovTheta<-solve(InfoMat)
> SE<-sqrt(diag(CovTheta))  #standard errors of parameter estimates
> theta
[1] 28.13688 12.57428
> MSE
[1] 0.2688919
```

```
> InfoMat
          [,1]      [,2]
[1,]  15.37455 -13.73842
[2,] -13.73842  13.92197
> CovTheta
          [,1]      [,2]
[1,] 0.5502797 0.5430248
[2,] 0.5430248 0.6076944
> SE
[1] 0.7418084 0.7795476
```

Hence, the parameter estimates are $\hat{\gamma}_0$ = 28.14 and $\hat{\gamma}_1$ = 12.57. The nls() script and output is as below, for which the estimates are the same.

```
> out2<-nls(y~p[1]*x/(p[2]+x),start=list(p=c(29.6,13.4)),data=Enz)
> summary(out2)

Formula: y ~ p[1] * x/(p[2] + x)

Parameters:
   Estimate Std. Error t value Pr(>|t|)
p1  28.1370     0.7280   38.65  < 2e-16 ***
p2  12.5745     0.7631   16.48 1.85e-11 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.5185 on 16 degrees of freedom

Number of iterations to convergence: 4
Achieved convergence tolerance: 4.479e-07

> logLik(out2)
'log Lik.' -12.65983 (df=3)
> vcov(out2)
          p1        p2
p1 0.5299534 0.5202828
p2 0.5202828 0.5822505
> confint.default(out2)
      2.5 %   97.5 %
p1 26.71024 29.56386
p2 11.07890 14.07001
```

3) Refer to the same data from Problem 13.10 of KNN.

(a) Calculate the observed Fisher information matrix and the covariance matrix of the estimated parameter vector $\hat{\boldsymbol{\gamma}} = [\hat{\gamma}_0, \hat{\gamma}_1]^T$ using the Hessian produced by nlm(). Based on this, calculate the standard errors of the estimated parameters.

See the R output from Problem 2 for calculations. For nonlinear LS with $\boldsymbol{\theta} = \boldsymbol{\gamma}$ (see notes),

$$log\ f(\mathbf{Y};\boldsymbol{\theta}) = \text{constant} - \frac{1}{2\hat{\sigma}^2}\sum_{i=1}^{n}[y_i - g(\mathbf{x}_i,\boldsymbol{\theta})]^2$$

$$\hat{\mathbf{I}}(\hat{\boldsymbol{\theta}}) = -\left.\frac{\partial^2 \log f(\mathbf{Y};\boldsymbol{\theta})}{\partial\boldsymbol{\theta}\partial\boldsymbol{\theta}^T}\right|_{\boldsymbol{\theta}=\hat{\boldsymbol{\theta}}} = \frac{1}{2\hat{\sigma}^2}\left.\frac{\partial^2 \sum_{i=1}^{n}[y_i - g(\mathbf{x}_i,\boldsymbol{\theta})]^2}{\partial\boldsymbol{\theta}\partial\boldsymbol{\theta}^T}\right|_{\boldsymbol{\theta}=\hat{\boldsymbol{\theta}}} = \frac{1}{2\hat{\sigma}^2}\,Hessian$$

$$= \begin{bmatrix} 15.37 & -13.74 \\ -13.74 & 13.92 \end{bmatrix}$$

where $\hat{\sigma}^2$ = MSE = 0.268

The covariance matrix is the inverse of the information matrix, i.e.,

$$Cov(\hat{\boldsymbol{\theta}}) = \hat{\mathbf{I}}^{-1}(\hat{\boldsymbol{\theta}}) = \begin{bmatrix} 0.550 & 0.543 \\ 0.543 & 0.608 \end{bmatrix}$$

and the standard errors are the square roots of the diagonal elements of the covariance matrix:

SE($\hat{\gamma}_0$) = 0.742
SE($\hat{\gamma}_1$) = 0.780

(b) Calculate the covariance matrix of $\hat{\boldsymbol{\gamma}}$ using the vcov() function applied to the output of nls(), and based on this calculate the standard errors of the estimated parameters. Do the results agree with Part (a)?

From the R output above,

$$Cov(\hat{\boldsymbol{\theta}}) = \hat{\mathbf{I}}^{-1}(\hat{\boldsymbol{\theta}}) = \begin{bmatrix} 0.530 & 0.520 \\ 0.520 & 0.582 \end{bmatrix},$$

from which the standard errors are

SE($\hat{\gamma}_0$) = 0.727

SE($\hat{\gamma}_1$) = 0.763

which is very close to part (a).

(c) Using the results of Part (a), calculate two-sided 95% CIs on the parameters γ_0 and γ_1. Compare this with the results of the confint.default() function applied to the output of nls().

For γ_0: $\hat{\gamma}_0 \pm z_{.025} SE(\hat{\gamma}_0) =$ 28.14 ± 1.96*0.742 = 28.14 ± 1.454 = [26.69, 29.59]
For γ_1: $\hat{\gamma}_1 \pm z_{.025} SE(\hat{\gamma}_1) =$ 12.57 ± 1.96*0.780 = 12.57 ± 1.529 = [11.04, 14.10]

For the nls() function, the CIs are:

```
> confint.default(out2)
      2.5 %   97.5 %
p1 26.71024 29.56386
p2 11.07890 14.07001
```

which are very close. The difference is probably due to the SEs being a little smaller for the nls() results.

4) This is a repeat of Problem (3), but using bootstrapping to calculate the standard errors and confidence intervals. You can use the boot() command in R (requires the boot package to be loaded with the library(boot) command). Use at least 20,000 bootstrap replicates.

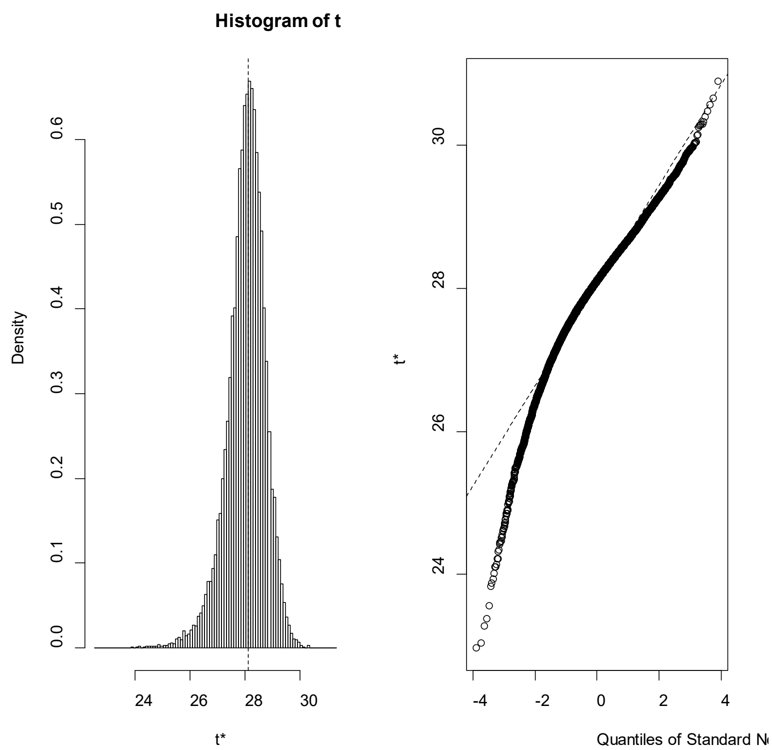
The R code and results for parts (a)—(c) are:

```
> library(boot)   #need to load the boot package
> Enzfit<-function(Z,i,theta0) {
+    Zboot<-Z[i,]
+    x<-Zboot[[2]];
+    y<-Zboot[[1]]
+    fn <- function(p) {yhat<-p[1]*x/(p[2]+x); sum((y-yhat)^2)}
+    out<-nlm(fn,p=theta0)
+    theta<-out$estimate}  #parameter estimates
> Enzboot<-boot(Enz, Enzfit, R=20000, theta0=c(29.6,13.4))
> CovTheta<-cov(Enzboot$t)
> SE<-sqrt(diag(CovTheta))
> Enzboot

ORDINARY NONPARAMETRIC BOOTSTRAP
```

```
Call:
boot(data = Enz, statistic = Enzfit, R = 20000, theta0 = c(29.6,
   13.4))


Bootstrap Statistics :
    original      bias    std. error
t1* 28.13688 -0.08920329   0.7040837
t2* 12.57428 -0.06325487   0.7331663
> CovTheta
          [,1]      [,2]
[1,] 0.4957338 0.4795740
[2,] 0.4795740 0.5375328
> SE
[1] 0.7040837 0.7331663
> plot(Enzboot,index=1)  #index=i calculates results for ith parameter
```

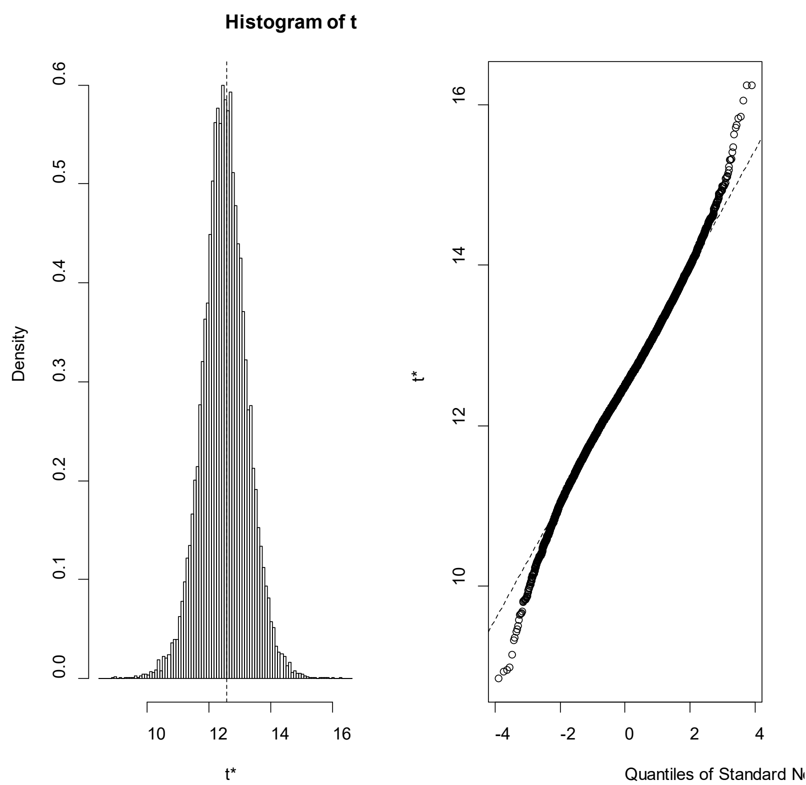



```
> boot.ci(Enzboot,conf=.95,index=1,type=c("norm","basic"))
BOOTSTRAP CONFIDENCE INTERVAL CALCULATIONS
Based on 20000 bootstrap replicates

CALL :
boot.ci(boot.out = Enzboot, conf = 0.95, type = c("norm", "basic"),
    index = 1)
```

Intervals :
Level   Normal   Basic
95%   (26.85, 29.61)   (27.02, 29.84)
Calculations and Intervals on Original Scale

> plot(Enzboot,index=2) #index=i calculates results for ith parameter



> boot.ci(Enzboot,conf=.95,index=2,type=c("norm","basic"))
BOOTSTRAP CONFIDENCE INTERVAL CALCULATIONS
Based on 20000 bootstrap replicates

CALL :
boot.ci(boot.out = Enzboot, conf = 0.95, type = c("norm", "basic"),
   index = 2)

Intervals :
Level   Normal   Basic
95%   (11.20, 14.07)   (11.18, 14.09)
Calculations and Intervals on Original Scale

(a) Calculate and plot bootstrapped histograms of $\hat{\gamma}_0$ and $\hat{\gamma}_1$, and calculate the corresponding bootstrapped standard errors.

The histograms and SEs are shown above. The SEs are

$$\text{SE}(\hat{\gamma}_0) = 0.704$$
$$\text{SE}(\hat{\gamma}_1) = 0.733$$

which are quite close to the results from Problem 3

(b) Calculate approximate two-sided 95% CIs on γ_0 and γ_1 using the normal approximation to their bootstrapped distributions.

For γ_0: $\hat{\gamma}_0 \pm z_{.025} SE(\hat{\gamma}_0) =$ 28.14 ± 1.96*0.704 = 28.14 ± 1.38 = [26.76, 29.51]
For γ_1: $\hat{\gamma}_1 \pm z_{.025} SE(\hat{\gamma}_1) =$ 12.57 ± 1.96*0.733 = 12.57 ± 1.44 = [11.13, 14.01]

These differ from the type = "normal" CIs calculated by boot.ci() only in that the latter subtracts the bias and calculates the CIs as:

$$\hat{\gamma}_j \pm z_{.025} SE(\hat{\gamma}_j) - BIAS(\hat{\gamma}_j)$$

(c) Calculate the reflected two-sided 95% CIs on γ_0 and γ_1 (this corresponds to the type = "basic" option of the boot.ci() function).

From the above results, the CIs are:

For γ_0: [27.02, 29.84]
For γ_1: [11.18, 14.09]

These are of the form $2\hat{\theta} - \hat{\theta}_{\alpha/2} \le \theta \le 2\hat{\theta} - \hat{\theta}_{1-\alpha/2}$

(d) Do the CIs in part (c) agree with those in part (b)? Relate this to the histograms you see in part (a).

They are somewhat different, mainly because the bootstrapped distributions are not centered about $\hat{\theta}$, especially for the γ_0 parameter.

5) Use bootstrapping to calculate a two-sided 95% prediction interval on a "future" response Y^* at $X^* = 27$. Compare this to a two-sided 95% confidence interval on the predictable part $g(\mathbf{x}^*, \boldsymbol{\theta})$ of Y^* at $X^* = 27$. Which interval do you think better represents an interval that you would expect to contain the future response with roughly 95% chance? Explain

The R code and results for the CI on $g(\mathbf{x}^*, \boldsymbol{\theta})$ are:

```
> Enzfit<-function(Z,i,theta0,x_pred) {
+   Zboot<-Z[i,]
+   x<-Zboot[[2]];
+   y<-Zboot[[1]]
+   fn <- function(p) {yhat<-p[1]*x/(p[2]+x); sum((y-yhat)^2)}
+   out<-nlm(fn,p=theta0)
+   theta<-out$estimate
+   y_pred<- theta[1]*x_pred/(theta[2]+x_pred)} #predicted response
> Enzboot<-boot(Enz, Enzfit, R=20000, theta0=c(29.6,13.4), x_pred=27)
> VarYhat<-var(Enzboot$t)
> SEYhat<-sqrt(VarYhat)
> Enzboot

ORDINARY NONPARAMETRIC BOOTSTRAP


Call:
boot(data = Enz, statistic = Enzfit, R = 20000, theta0 = c(29.6,
   13.4), x_pred = 27)


Bootstrap Statistics :
   original      bias    std. error
t1* 19.19671 -0.03116383   0.2049908
> VarYhat
           [,1]
[1,] 0.04202122
> SEYhat
          [,1]
[1,] 0.2049908
> plot(Enzboot)
> boot.ci(Enzboot,conf=.95,type=c("norm","basic"))
BOOTSTRAP CONFIDENCE INTERVAL CALCULATIONS
Based on 20000 bootstrap replicates

CALL :
boot.ci(boot.out = Enzboot, conf = 0.95, type = c("norm", "basic"))

Intervals :
Level      Normal              Basic
95%   (18.83, 19.63 )   (18.91, 19.71 )
Calculations and Intervals on Original Scale
```

Additional R code and results for the PI on are:

```
> Yhat0<-Enzboot$t0
> Yhatboot<-Enzboot$t
> e<-rnorm(nrow(Yhatboot), mean=0, sd=sqrt(MSE))
> Yboot<-Yhatboot+e
> SEY<-sqrt(var(Yboot))
> Yquant<-quantile(Yboot,prob=c(.025,.975))
> L<-2*Yhat0-Yquant[2]
> U<-2*Yhat0-Yquant[1]
> c(L,U)
   97.5%     2.5%
18.14644 20.33650
> SEY
          [,1]
[1,] 0.5570887
```

From the above, the reflected CI and PI (corresponding to type = "basic") are:

CI on $g(\mathbf{x}^*,\boldsymbol{\theta})$: [18.91, 19.71]
PI on Y^*: [18.15, 20.34]

6) Use the AIC criterion to compare the model that you fitted in Problem (2) with the alternative model $Y_i = \beta_0 + \beta_1\sqrt{X_i} + \varepsilon_i$. Which model does AIC suggest is the better model?

From Problem 2, the SSE = 4.3023, and the log-likelihood is logLik(out2) = -12.65983 (or compute it from the expression given). Hence

$$AIC = \frac{-2\,log\, f(\mathbf{y};\hat{\boldsymbol{\theta}})}{n} + \frac{2p}{n} = \frac{-2(-12.66)}{18} + \frac{2(2)}{18} = 1.629$$

For the new model, we can simply fit a linear regression model using the lm() command in R, as follows:

```
> out3<-lm(y~sqrt(x),data=Enz)
> summary(out3)

Call:
lm(formula = y ~ sqrt(x), data = Enz)

Residuals:
    Min      1Q  Median      3Q     Max
-1.7997 -0.5451  0.2085  0.4413  1.6771

Coefficients:
```

```
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  -0.4566     0.5154  -0.886    0.389
sqrt(x)       3.7720     0.1401  26.918 9.41e-15 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.9483 on 16 degrees of freedom
Multiple R-squared: 0.9784,     Adjusted R-squared: 0.977
F-statistic: 724.6 on 1 and 16 DF,  p-value: 9.414e-15
```

The SSE = 14.3883, and the log-likelihood is (from the expression given, or from below) is:

```
> logLik(out3)
'log Lik.' -23.52533 (df=3)
```

Thus,

$$AIC = \frac{-2\,log\,f(\mathbf{y};\hat{\boldsymbol{\theta}})}{n} + \frac{2p}{n} = \frac{-2(-23.53)}{18} + \frac{2(2)}{18} = 2.836$$

Since this is much larger than for the Problem 2 model, we conclude the model from Problem 2 is better.

7) Use n-fold cross-validation to compare the model that you fitted in Problem (2) with the alternative model $Y_i = \beta_0 + \beta_1 \sqrt{X_i} + \varepsilon_i$. Which model does n-fold cross-validation suggest is the better model?

The R code and results for n-fold CV for the Problem 2 model is:

```
> Enz<-read.table("Enz.csv",sep=",",header=TRUE)
> n<-nrow(Enz)
> K<-n
> m<-floor(n/K)  #approximate size of each part
> r<-n-m*K
> I<-sample(n,n)  #random reordering of the indices
> FitFun <- function(x,p) p[1]*x/(p[2]+x)
> SSE<-0
> for (k in 1:K) {
+   if (k <= r) kpart <- ((m+1)*(k-1)+1):((m+1)*k)
+     else kpart<-((m+1)*r+m*(k-r-1)+1):((m+1)*r+m*(k-r))
+   Itest <- I[kpart]  #indices for kth part of data
+   Itrain <- I[-kpart]  #indices for everything but kth part of data
+   Xtrain<-Enz[Itrain,]  #training data for kth part
+   Xtest<-Enz[Itest,]  #test data for kth part
+   out<-nls(y~FitFun(x,p),data=Xtrain,start=list(p=c(29.6,13.4)))
```

```
+   Yhat<-predict(out,Xtest)
+   SSE<-SSE+sum((Xtest$y-Yhat)^2)
+ }
> SSE
[1] 5.297425
```

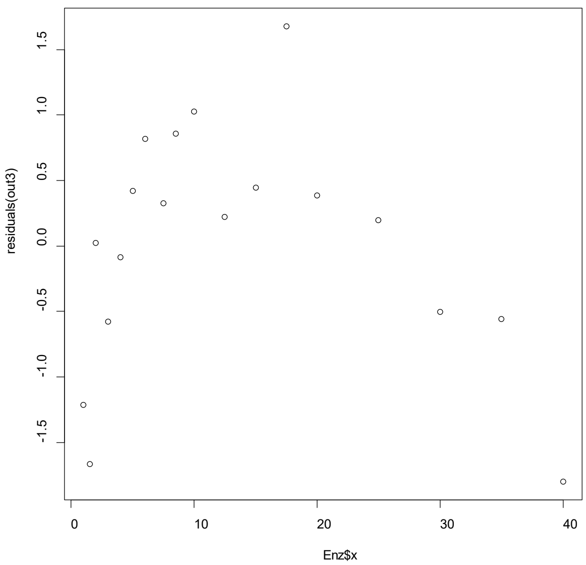
Analogous R code and results for n-fold CV for the new model is:

```
> Enz<-read.table("Enz.csv",sep=",",header=TRUE)
> n<-nrow(Enz)
> K<-n
> m<-floor(n/K)  #approximate size of each part
> r<-n-m*K
> I<-sample(n,n)  #random reordering of the indices
> SSE<-0
> for (k in 1:K) {
+   if (k <= r) kpart <- ((m+1)*(k-1)+1):((m+1)*k)
+      else kpart<-((m+1)*r+m*(k-r-1)+1):((m+1)*r+m*(k-r))
+   Itest <- I[kpart]  #indices for kth part of data
+   Itrain <- I[-kpart]  #indices for everything but kth part of data
+   Xtrain<-Enz[Itrain,]  #training data for kth part
+   Xtest<-Enz[Itest,]  #test data for kth part
+   out<-lm(y~sqrt(x),data=Xtrain)
+   Yhat<-predict(out,Xtest)
+   SSE<-SSE+sum((Xtest$y-Yhat)^2)
+ }
> SSE
[1] 19.99179
```

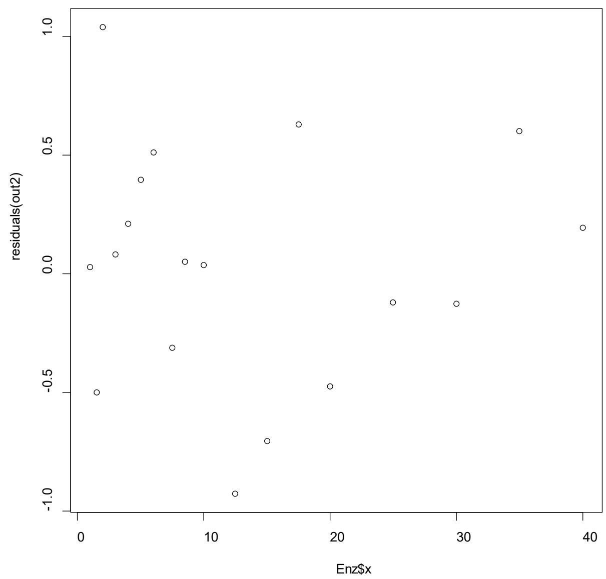
The CV SSEs are 5.297 for the Problem 2 model versus 19.992 for the new model. Hence, the Problem 2 model is clearly much better.

8) For the two models that you compared in Problems 6 and 7, construct plots of the residuals versus *X*. Based on the residual plots, does one model appear more appropriate than the other, and does this agree with your conclusions from Problems 6 and 7?

The residuals for the new model of problems 6 and 7 (left plot) and for the model of Problem 2 (right plot) are below. Clearly the residuals for the Problem 2 model are more random and have smaller variance. Hence the conclusion is the same (Problem 2 model is better).



residuals(out3)
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
0
10
20
30
40
Enz$x



residuals(out2)
1.0
0.5
0.0
-0.5
-1.0
0
10
20
30
40
Enz$x