

hw5

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```
library('MASS') ## for 'mcycle'
library('manipulate') ## for 'manipulate'
library(dplyr)
```

```
##
## Attaching package: 'dplyr'
```

```
## The following object is masked from 'package:MASS':
##
##      select
```

```
## The following objects are masked from 'package:stats':
##
##      filter, lag
```

```
## The following objects are masked from 'package:base':
##
##      intersect, setdiff, setequal, union
```

```
library(caret)
```

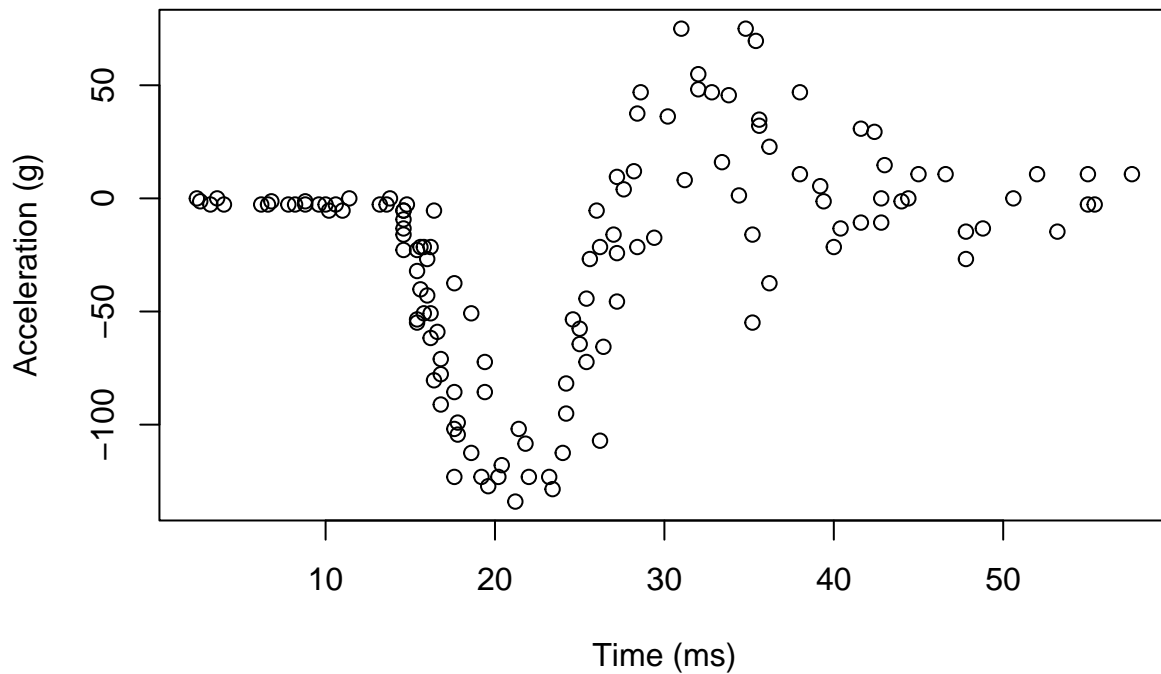
```
## Loading required package: ggplot2
```

```
## Loading required package: lattice
```

```
library("knitr")
```

```
y <- mcycle$accel
x <- matrix(mcycle$times, length(mcycle$times), 1)

plot(x, y, xlab="Time (ms)", ylab="Acceleration (g)")
```



Question 1: Randomly split the mcycle data into training (75%) and validation (25%) subsets

```
train_data<-sample_frac(mcycle, 0.75)
sid<-as.numeric(rownames(train_data))
test_data<-mcycle[-sid,]
```

```
sid
```

```
##      [1]      1      2      3      4      5      6      7      8      9     10     11     12     13     14     15     16     17     18
##    [19]     19     20     21     22     23     24     25     26     27     28     29     30     31     32     33     34     35     36
##   [37]     37     38     39     40     41     42     43     44     45     46     47     48     49     50     51     52     53     54
##  [55]     55     56     57     58     59     60     61     62     63     64     65     66     67     68     69     70     71     72
##  [73]     73     74     75     76     77     78     79     80     81     82     83     84     85     86     87     88     89     90
##  [91]     91     92     93     94     95     96     97     98     99    100
```

```
test_data
```

```
##      times accel
## 101    35.2  -16.0
## 102    35.2  -54.9
## 103    35.4   69.6
## 104    35.6   34.8
## 105    35.6   32.1
## 106    36.2  -37.5
## 107    36.2   22.8
## 108    38.0   46.9
## 109    38.0   10.7
## 110    39.2    5.4
```

```
## 111 39.4 -1.3
## 112 40.0 -21.5
## 113 40.4 -13.3
## 114 41.6 30.8
## 115 41.6 -10.7
## 116 42.4 29.4
## 117 42.8 0.0
## 118 42.8 -10.7
## 119 43.0 14.7
## 120 44.0 -1.3
## 121 44.4 0.0
## 122 45.0 10.7
## 123 46.6 10.7
## 124 47.8 -26.8
## 125 47.8 -14.7
## 126 48.8 -13.3
## 127 50.6 0.0
## 128 52.0 10.7
## 129 53.2 -14.7
## 130 55.0 -2.7
## 131 55.0 10.7
## 132 55.4 -2.7
## 133 57.6 10.7
```

Question 2: Using the mcycle data, consider predicting the mean acceleration as a function of time

```
## Epanechnikov kernel function
## x - n x p matrix of training inputs
## x0 - 1 x p input where to make prediction
## lambda - bandwidth (neighborhood size)
kernel_epanechnikov <- function(x, x0, lambda=1) {
  d <- function(t)
    ifelse(t <= 1, 3/4*(1-t^2), 0)
  z <- t(t(x) - x0)
  d(sqrt(rowSums(z*z))/lambda)
}

## k-NN kernel function
## x - n x p matrix of training inputs
## x0 - 1 x p input where to make prediction
## k - number of nearest neighbors
kernel_k_nearest_neighbors <- function(x, x0, k=1) {
  ## compute distance between each x and x0
  z <- t(t(x) - x0)
  d <- sqrt(rowSums(z*z))

  ## initialize kernel weights to zero
  w <- rep(0, length(d))

  ## set weight to 1 for k nearest neighbors
  w[order(d)[1:k]] <- 1
}
```

```

    return(w)
}

## Make predictions using the NW method
## y - n x 1 vector of training outputs
## x - n x p matrix of training inputs
## x0 - m x p matrix where to make predictions
## kern - kernel function to use
## ... - arguments to pass to kernel function
nadaraya_watson <- function(y, x, x0, kern, ...) {
  k <- t(apply(x0, 1, function(x0_) {
    k_ <- kern(x, x0_, ...)
    k_/sum(k_)
  })))
  yhat <- drop(k %*% y)
  attr(yhat, 'k') <- k
  return(yhat)
}

## Helper function to view kernel (smoother) matrix
matrix_image <- function(x) {
  rot <- function(x) t(apply(x, 2, rev))
  cls <- rev(gray.colors(20, end=1))
  image(rot(x), col=cls, axes=FALSE)
  xlb <- pretty(1:ncol(x))
  xat <- (xlb-0.5)/ncol(x)
  ylb <- pretty(1:nrow(x))
  yat <- (ylb-0.5)/nrow(x)
  axis(3, at=xat, labels=xlb)
  axis(2, at=yat, labels=ylb)
  mtext('Rows', 2, 3)
  mtext('Columns', 3, 3)
}

## Compute effective df using NW method
## y - n x 1 vector of training outputs
## x - n x p matrix of training inputs
## kern - kernel function to use
## ... - arguments to pass to kernel function
effective_df <- function(y, x, kern, ...) {
  y_hat <- nadaraya_watson(y, x, x,
    kern=kern, ...)
  sum(diag(attr(y_hat, 'k'))))
}

```

Question 3: With the squared-error loss function, compute and plot the training error, AIC, BIC, and validation error

```

## loss function
## y - train/test y
## yhat - predictions at train/test x
loss_squared_error <- function(l_y, l_yhat)

```

```

(l_y - l_yhat)^2

## test/train error
## y      - train/test y
## yhat   - predictions at train/test x
## loss   - loss function
error <- function(l_y, l_yhat, loss=loss_squared_error)
  mean(loss(l_y, l_yhat))

## AIC
## y      - training y
## yhat   - predictions at training x
## d      - effective degrees of freedom
aic <- function(l_y, l_yhat, d)
  error(l_y, l_yhat) + 2/length(l_y)*d

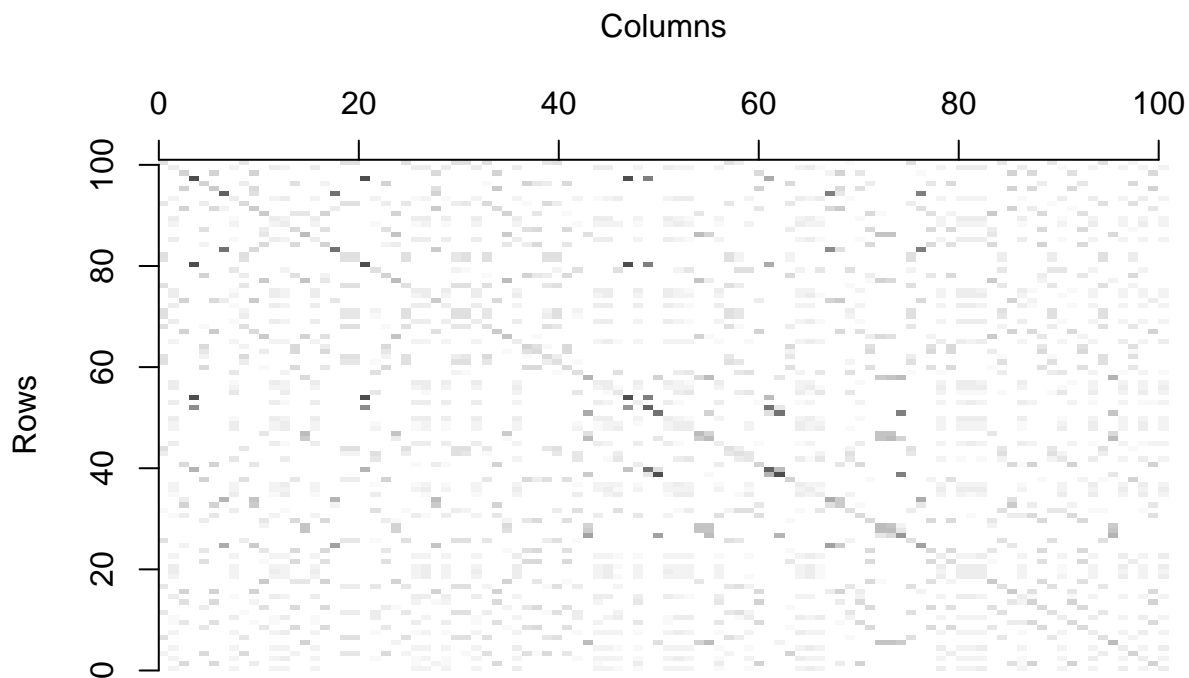
## BIC
## y      - training y
## yhat   - predictions at training x
## d      - effective degrees of freedom
bic <- function(l_y, l_yhat, d)
  error(l_y, l_yhat) + log(length(l_y))/length(l_y)*d

y <- train_data$accel
x <- matrix(train_data$times, length(train_data$times), 1)

## make predictions using NW method at training inputs
y_hat <- nadaraya_watson(y, x, x,
  kernel_epanechnikov, lambda=5)

## view kernel (smoother) matrix
matrix_image(attr(y_hat, 'k'))

```



```
## compute effective degrees of freedom
edf <- effective_df(y, x, kernel_epanechnikov, lambda=5)

## create a grid of inputs
x_plot <- matrix(seq(min(x),max(x),length.out=100),100,1)

## make predictions using NW method at each of grid points
y_hat_plot <- nadaraya_watson(y, x, x_plot,
  kernel_epanechnikov, lambda=1)
```

```
# Training Error
error(y, y_hat)
```

```
## [1] 746.4909
```

```
# AIC
aic(y, y_hat, edf)
```

```
## [1] 746.6594
```

```
# BIC
bic(y, y_hat, edf)
```

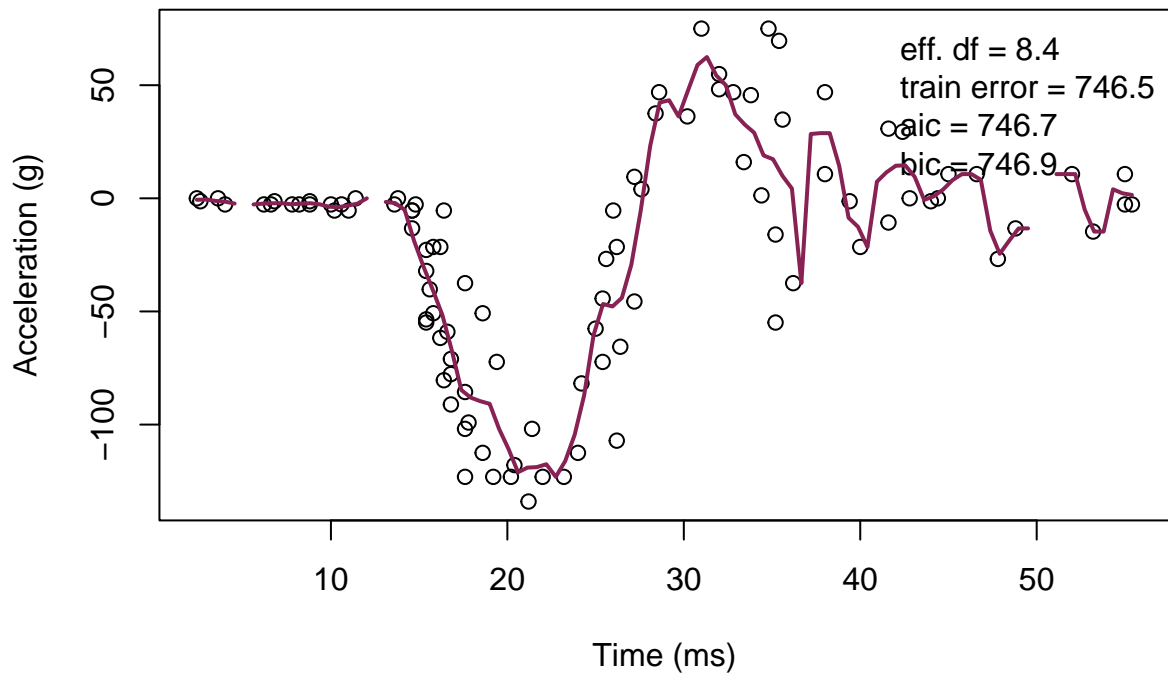
```
## [1] 746.8789
```

```
err<-error(y, y_hat)
aic_ <- aic(y, y_hat, edf)
bic_ <- bic(y, y_hat, edf)
```

```

plot(x, y, xlab="Time (ms)", ylab="Acceleration (g)")
  legend('topright', legend = c(
    paste0('eff. df = ', round(edf,1)),
    paste0('train error = ', round(err, 1)),
    paste0('aic = ', round(aic_, 1)),
    paste0('bic = ', round(bic_, 1))),
    bty='n')
lines(x_plot, y_hat_plot, col="#882255", lwd=2)

```



```

ky <- test_data$accel
kx <- matrix(test_data$times, length(test_data$times), 1)

## make predictions using NW method at testing inputs
ky_hat <- nadaraya_watson(ky, kx, kx,
  kernel_epanechnikov, lambda=5)

## compute effective degrees of freedom
# tedf <- effective_df(ty, tx, kernel_epanechnikov, lambda=5)

## create a grid of inputs
kx_plot <- matrix(seq(min(kx),max(kx),length.out=100),100,1)

## make predictions using NW method at each of grid points
ky_hat_plot <- nadaraya_watson(ky, kx, kx_plot,
  kernel_epanechnikov, lambda=1)

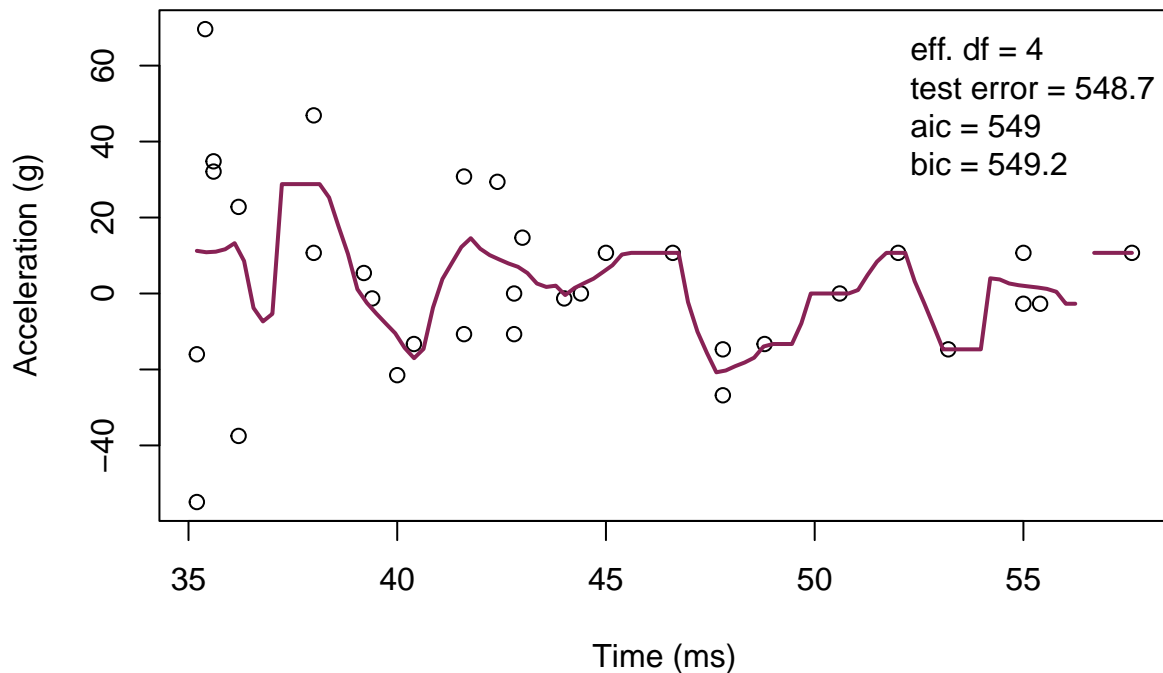
# Validation Error
err1<-error(ky, ky_hat)
kedf <- effective_df(ky, kx, kernel_epanechnikov, lambda=5)
# AIC

```

```

aic_<-aic(ky, ky_hat, kedf)
# BIC
bic_<-bic(ky, ky_hat, kedf)
## plot predictions
plot(kx, ky, xlab="Time (ms)", ylab="Acceleration (g)")
lines(kx_plot, ky_hat_plot, col="#882255", lwd=2)
legend('topright', legend = c(
  paste0('eff. df = ', round(kedf,1)),
  paste0('test error = ', round(err1, 1)),
  paste0('aic = ', round(aic_, 1)),
  paste0('bic = ', round(bic_, 1))),
  bty='n')

```



Question 4: For each value of the tuning parameter, Perform 5-fold cross-validation using the combined training and validation data. This results in 5 estimates of test error per tuning parameter value

```

set.seed(15)
mcycle_flds <- createFolds(mcycle$accel, k=5)
print(mcycle_flds)

```

```

## $Fold1
## [1] 5 7 8 10 24 25 26 34 37 40 41 44 56 60 64 67 85 88 89
## [20] 92 96 101 102 106 126 130 131
##
## $Fold2
## [1] 4 13 15 16 21 27 30 33 39 46 49 54 63 70 72 73 76 86 95
## [20] 97 98 104 115 119 120 125

```



```
##
## $Fold3
## [1] 9 12 17 20 22 29 31 32 42 47 58 61 62 68 79 80 81 83 91
## [20] 94 99 103 111 122 123 129 132
##
## $Fold4
## [1] 1 18 19 23 35 36 52 53 55 59 69 71 74 75 78 107 108 110 112
## [20] 114 118 121 124 127 128 133
##
## $Fold5
## [1] 2 3 6 11 14 28 38 43 45 48 50 51 57 65 66 77 82 84 87
## [20] 90 93 100 105 109 113 116 117
```

```
sapply(mcycle_flds, length)
```

```
## Fold1 Fold2 Fold3 Fold4 Fold5
## 27 26 27 26 27
```

```
cvknnreg_mcycle <- function(kNN = 10, flds=mcycle_flds) {
  cverr <- rep(NA, length(flds))
  for(tst_idx in 1:length(flds)) { ## for each fold

    ## get training and testing data
    mcycle_trn <- mcycle[-flds[[tst_idx]],]
    mcycle_tst <- mcycle[ flds[[tst_idx]],]

    ## fit kNN model to training data
    knn_fit <- knnreg(accel ~ times,
                      k=kNN, data=mcycle_trn)

    ## compute test error on testing data
    pre_tst <- predict(knn_fit, mcycle_tst)
    cverr[tst_idx] <- mean((mcycle_tst$accel - pre_tst)^2)
  }
  return(cverr)
}
```

Question 5: Plot the CV-estimated test error (average of the five estimates from each fold) as a function of the tuning parameter. Add vertical line segments to the figure (using the segments function in R) that represent one “standard error” of the CV-estimated test error

```
cverrs <- sapply(1:40, cvknnreg_mcycle)
print(cverrs)
```

```
##           [,1]      [,2]      [,3]      [,4]      [,5]      [,6]      [,7]
## [1,] 1714.2741 1225.5741 1194.6940 1288.9915 1276.1731 1171.3820 1184.8180
## [2,]  519.1238  269.7850  185.5025  268.1531  260.6804  233.1877  202.9172
## [3,] 1110.6328  686.9212  556.4522  522.7368  439.1764  467.2601  467.2058
## [4,]  971.6179  691.7369  655.7638  628.8749  631.2647  656.4100  594.0081
```

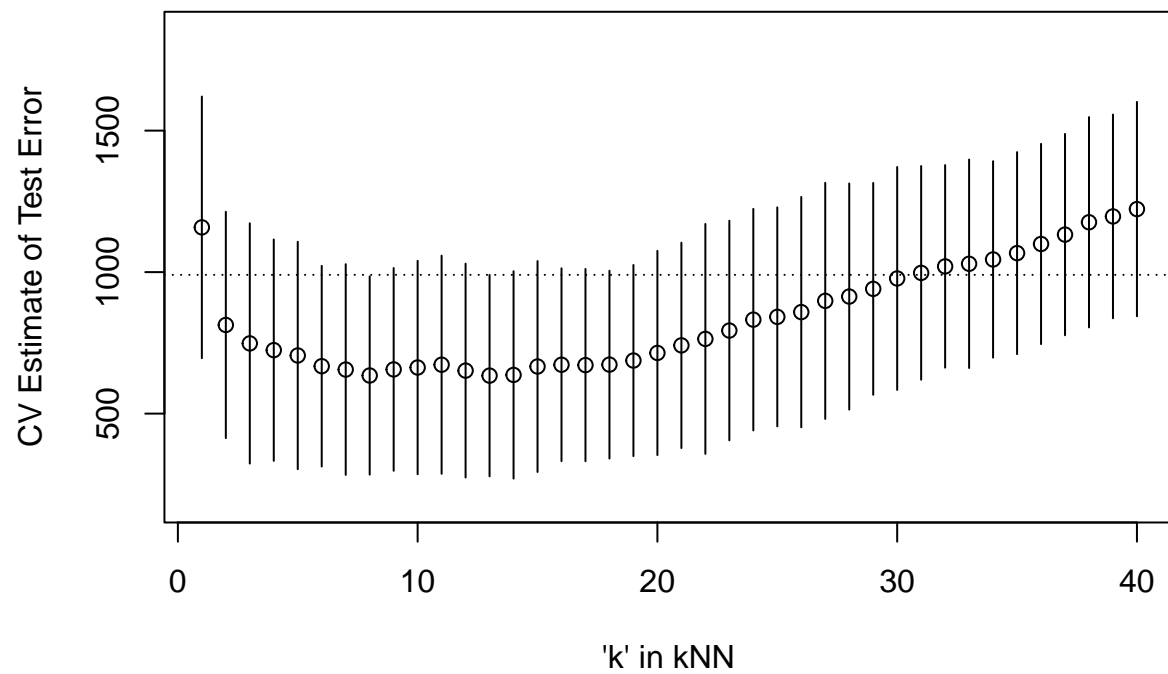
```
## [5,] 1474.8920 1192.2785 1148.2494 912.7228 920.2319 809.7640 829.7366
##      [,8]      [,9]      [,10]      [,11]      [,12]      [,13]      [,14]
## [1,] 1128.8391 1179.7252 1247.7534 1279.9892 1258.2631 1193.1744 1218.2526
## [2,] 182.1323 217.6144 243.7948 244.6061 234.0310 220.4289 215.2597
## [3,] 479.3272 485.8238 463.7354 478.1474 484.8418 487.1394 500.6296
## [4,] 615.3839 614.8452 606.3356 635.2262 618.5401 605.0913 588.8028
## [5,] 767.6451 782.9823 753.1773 725.9601 663.8392 665.5412 660.8071
##      [,15]      [,16]      [,17]      [,18]      [,19]      [,20]      [,21]
## [1,] 1255.8161 1212.6865 1209.2418 1203.7611 1232.5108 1296.6235 1328.4156
## [2,] 238.0875 282.9021 274.1647 291.1334 301.3908 301.0971 328.9239
## [3,] 532.4641 537.3451 551.2119 562.6586 600.5497 626.4130 648.1937
## [4,] 596.4829 629.4134 654.5002 641.6799 652.3628 660.9103 690.6735
## [5,] 709.5163 701.0754 668.0268 666.7256 651.1609 687.0429 709.9031
##      [,22]      [,23]      [,24]      [,25]      [,26]      [,27]      [,28]
## [1,] 1444.9842 1447.9111 1502.9871 1507.2693 1566.1316 1613.5059 1587.4674
## [2,] 355.1384 410.8127 473.6967 493.8207 520.0545 529.1936 522.9638
## [3,] 624.9934 663.8973 717.2165 711.4466 706.8416 759.5581 792.9546
## [4,] 676.5652 699.8368 704.9470 731.6596 730.1856 731.0626 787.2829
## [5,] 718.4453 745.1866 761.6988 765.3411 770.3431 858.9445 877.8209
##      [,29]      [,30]      [,31]      [,32]      [,33]      [,34]      [,35]
## [1,] 1573.1530 1650.8496 1638.8546 1627.6508 1655.7542 1629.5808 1676.0561
## [2,] 577.2849 620.6617 640.5730 689.7478 689.2437 722.9051 774.2112
## [3,] 810.5431 825.8785 868.3449 890.5762 936.0847 956.0453 987.5866
## [4,] 841.6003 853.8440 882.1799 889.1085 871.2455 876.1727 852.2868
## [5,] 901.5220 936.6488 956.6900 1003.9637 994.9708 1039.3533 1045.6052
##      [,36]      [,37]      [,38]      [,39]      [,40]
## [1,] 1701.0613 1726.500 1792.8060 1806.3105 1853.1714
## [2,] 796.6132 807.597 841.9857 916.4554 931.1676
## [3,] 1044.1188 1087.715 1162.1688 1159.4262 1180.7908
## [4,] 892.8485 918.675 932.1466 940.5811 922.9947
## [5,] 1062.4498 1122.771 1151.9358 1161.3120 1225.4667
```

```
cverrs_mean <- apply(cverrs, 2, mean)
cverrs_sd   <- apply(cverrs, 2, sd)

plot(x=1:40, y=cverrs_mean,
     ylim=range(cverrs),
     xlab="'k' in kNN", ylab="CV Estimate of Test Error")
segments(x0=1:40, x1=1:40,
         y0=cverrs_mean-cverrs_sd,
         y1=cverrs_mean+cverrs_sd)
best_idx <- which.min(cverrs_mean)
points(x=best_idx, y=cverrs_mean[best_idx], pch=30)
```

```
## Warning in plot.xy(xy.coords(x, y), type = type, ...): unimplemented pch value
## '30'
```

```
abline(h=cverrs_mean[best_idx] + cverrs_sd[best_idx], lty=3)
```



Question 6: Interpret the resulting figures and select a suitable value for the tuning parameter.

It is reasonable for the tuning parameter to be 30, $k=30$