Multiple Regression by Linear Algebra

We previously considered the following observations $Y_1, Y_2, \ldots, Y_n$ following linear model $E(Y) = \beta_0 + \beta_1 x$:

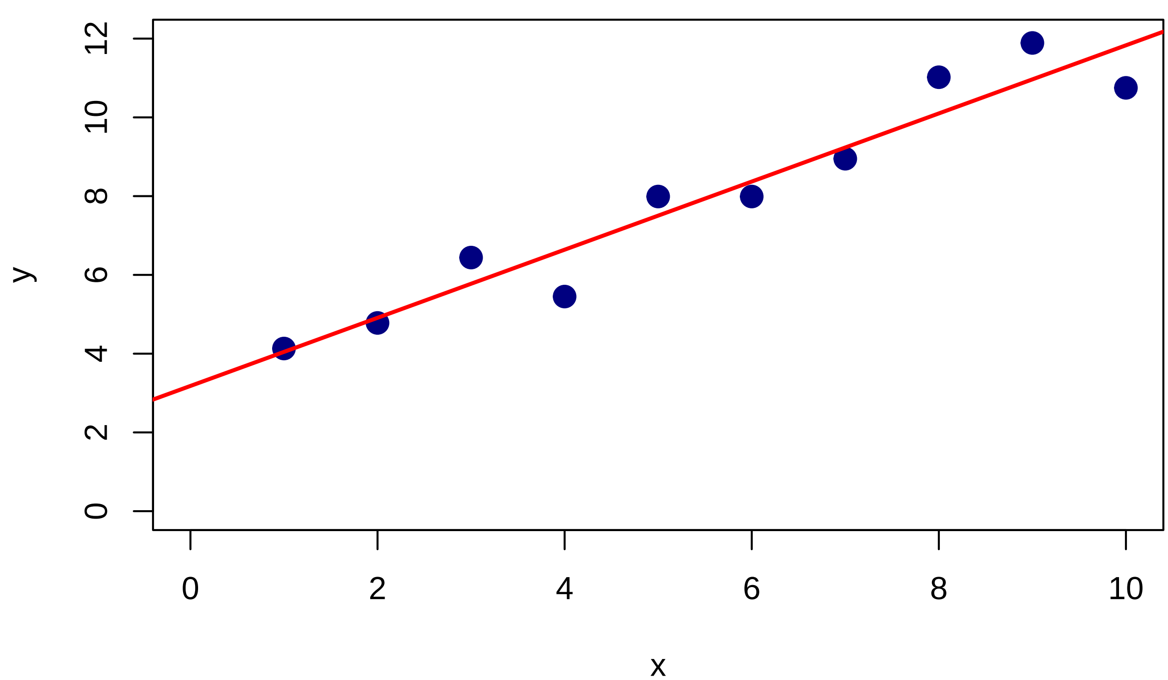
x	1	2	3	4	5	6	7	8	9	10
y	4.13	4.78	6.44	5.45	7.99	7.99	8.95	11.02	11.89	10.75

In an earlier example, we fit the least squares model

$$\hat{y} = 3.18 + 0.865x$$

The following code plots each point (x, y) in the plane as well as the least squares model line. We can plot the fitted line, as well as the observed data using the **abline** function, which plots a line with given slope and intercept.

```
x <- 1:10
y <-  c(4.13,  4.78,  6.44,  5.45,  7.99,  7.99,  8.95, 11.02, 11.89, 10.75)
plot(x, y, xlim = c(0,10), ylim = c(0,12), col = "navy", pch = 19, cex = 1.5)
abline(3.18, 0.865, col = "red", lwd = 2)
```



Least Squares via Matrix Algebra

We could also have fit the least-squares line by solving the linear system

$$(\mathbf{X}'\mathbf{X})\hat{\boldsymbol{\beta}} = \mathbf{X}'\mathbf{Y},$$

where

$$\mathbf{Y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}, \qquad \mathbf{X} = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix}, \qquad \hat{\boldsymbol{\beta}} = \begin{bmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \end{bmatrix}.$$

We can create the coefficient matrices $\mathbf{X}'\mathbf{Y}$ and $\mathbf{X}'\mathbf{X}$ using the following code.

```
# Store X as matrix.
n <- length(x)
X = cbind(rep(x = 1, times = n), x)

# Form coefficient matrices.
XX = t(X) %*% X
XY = t(X) %*% y
```

Here, the function **t(X)** yields the transpose of the matrix $\mathbf{X}$ and the operator $\% * \%$ is used to perform matrix-matrix multiplication. This gives the matrices:

$$\mathbf{X}'\mathbf{X} = \begin{bmatrix} 10 & 55 \\ 55 & 385 \end{bmatrix} \qquad \mathbf{X}'\mathbf{Y} = \begin{bmatrix} 79.39 \\ 508.02 \end{bmatrix}$$

Solving using Matrix Inversion

There are several equivalent processes for solving the linear system $(\mathbf{X}'\mathbf{X})\hat{\boldsymbol{\beta}} = \mathbf{X}'\mathbf{Y}$. For example, we could calculate the inverse $(\mathbf{X}'\mathbf{X})^{-1}$ and evaluate

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}.$$

We can calculate the inverse $(\mathbf{X}'\mathbf{X})^{-1}$ using R function **solve** and calculate $\hat{\boldsymbol{\beta}}$ using the following code.

```
# Calculate inverse.
invXX <- solve(XX)

# Solve for hatbeta
hBeta <- invXX %*% XY
```

$$(\mathbf{X}'\mathbf{X})^{-\mathbf{1}} = \begin{bmatrix} 0.466666666666667 & -0.0666666666666667 \\ -0.0666666666666667 & 0.0121212121212121 \end{bmatrix} \qquad \hat{\boldsymbol{\beta}} = \begin{bmatrix} 3.18066666666667 \\ 0.865151515151515 \end{bmatrix}$$

Note that the entries of $\hat{\boldsymbol{\beta}}$ agree with the values of the $\hat{\beta}_0$ and $\hat{\beta}_1$ calculated earlier.

Solving via Gaussian Elimination

We can also solve the system $(\mathbf{X}'\mathbf{X})\hat{\boldsymbol{\beta}} = \mathbf{X}'\mathbf{Y}$ by reducing the augmented matrix

$$\begin{bmatrix} \mathbf{X}'\mathbf{X} & \mathbf{X}'\mathbf{Y} \end{bmatrix}$$

to reduced row echelon form using Gaussian elimination. The resulting matrix will have final column equal to $\hat{\boldsymbol{\beta}}$. The following code uses the R function **rref** (part of the **pracma** package) to perform the necessary elementary row operations.

```r
# Load pracma package.
library(pracma)

# Form augmented matrix.
Ab <- cbind(XX, XY)

# Reduce to RREF.
rrefAB <- rref(Ab)
```

$$\begin{bmatrix} 10 & 55 & 79.39 \\ 55 & 385 & 508.02 \end{bmatrix} \sim \begin{bmatrix} 1 & 0 & 3.18066666666667 \\ 0 & 1 & 0.865151515151515 \end{bmatrix}$$

Notice that the final column of the reduced matrix agrees with the value of $\hat{\boldsymbol{\beta}}$ calculated the using the **inv** function and the values of $\hat{\beta}_0$ and $\hat{\beta}_1$ calculated directly using the least-squares equations.

Using the Solve Function

We can also use the **solve** function to solve the linear system for the least squares estimator using Gaussian elimination (without explicitly forming the inverse $(\mathbf{X}'\mathbf{X})^{-1}$. Indeed, the command **solve(A,b)** calls R's linear system solving routines (based on the LAPACK package https://www.netlib.org/lapack/) to solve the system $\mathbf{A}\mathbf{x} = \mathbf{b}$. This syntax differs from our earlier use of **solve(XX)**: the command **solve(A)** yields the inverse of the matrix **A** when given a single matrix argument as input. The following code specializes the process to solving the least-squares system.

```r
hBetaS <- solve(XX, XY)
```

This yields

$$\hat{\boldsymbol{\beta}} = \begin{bmatrix} 3.18066666666667 \\ 0.865151515151515 \end{bmatrix}$$

Note that this gives the same least-squares estimators as before (as should be expected).

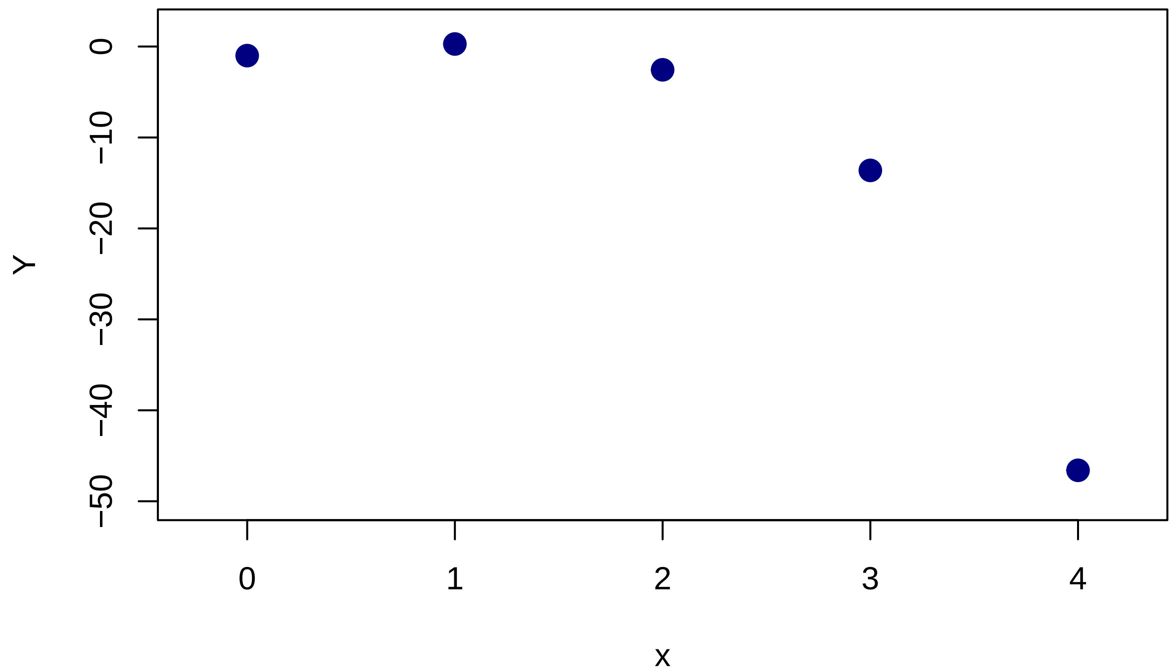
A Nonlinear Example

Suppose that the response variable Y follows the model:

$$Y = \beta_0 + \beta_1 x + \beta_2 \sqrt{x} + \beta_3 e^x + \epsilon..$$

We have the following observations:

x	0	1	2	3	4
y	-1.00	0.28	-2.56	-13.62	-46.60



We can calculate the least squares estimates $\hat{\beta}_0, \hat{\beta}_1, \hat{\beta}_2, \hat{\beta}_3$ by solving the linear system

$$(\mathbf{X}'\mathbf{X})\hat{\boldsymbol{\beta}} = \mathbf{X}'\mathbf{Y},$$

where

$$\mathbf{X} = \begin{bmatrix} 1 & x_1 & \sqrt{x_1} & e^{x_1} \\ 1 & x_2 & \sqrt{x_2} & e^{x_2} \\ \vdots & \vdots & \vdots & \vdots \\ 1 & x_n & \sqrt{x_n} & e^{x_n} \end{bmatrix}, \qquad \mathbf{Y} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}, \qquad \hat{\boldsymbol{\beta}} = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \beta_3 \end{bmatrix}.$$

The following code creates $\mathbf{X}$ and $\mathbf{Y}$ for the given data.

```
# Load data.
x2 <- 0:4
y2 <- c(-1, 0.28, -2.56, -13.62, -46.60)
n2 <- length(x2)
# Create X.
X2 <- cbind(rep(x = 1, times = n2), x2, sqrt(x2), exp(x2))
```

This gives following the matrix $\boldsymbol{X}$ of independent variable values.

$$\mathbf{X} = \begin{bmatrix} 1 & 0 & 0 & 1 \\ 1 & 1 & 1 & 2.71828182845905 \\ 1 & 2 & 1.4142135623731 & 7.38905609893065 \\ 1 & 3 & 1.73205080756888 & 20.0855369231877 \\ 1 & 4 & 2 & 54.5981500331442 \end{bmatrix}.$$

After forming $\mathbf{X}$, we can create the coefficient matrices $\mathbf{X}'\mathbf{X}$ and $\mathbf{X}'\mathbf{Y}$ for the least squares linear system using the following code.

```r
XX2 <- t(X2) %*% X2
XY2 <- t(X2) %*% y2
```

$$\mathbf{X}'\mathbf{X} = \begin{bmatrix} 5 & 10 & 6.14626436994197 & 85.7910248837216 \\ 10 & 30 & 17.0245795474528 & 296.14560492846 \\ 6.14626436994197 & 17.0245795474528 & 10 & 157.153455691253 \\ 85.7910248837216 & 296.14560492846 & 157.153455691253 & 3447.37398666654 \end{bmatrix}$$

$$\mathbf{X}'\mathbf{Y} = \begin{bmatrix} -63.5 \\ -232.1 \\ -120.130918718763 \\ -2836.99366913963 \end{bmatrix}$$

We're ready to calculate $\hat{\boldsymbol{\beta}}$ using the **solve** function.

```r
hBetaN <- solve(XX2, XY2)
```

$$\hat{\boldsymbol{\beta}} = \begin{bmatrix} 0.000213940602612812 \\ 1.00627266650045 \\ 1.99247632462577 \\ -1.00022214125921 \end{bmatrix}$$

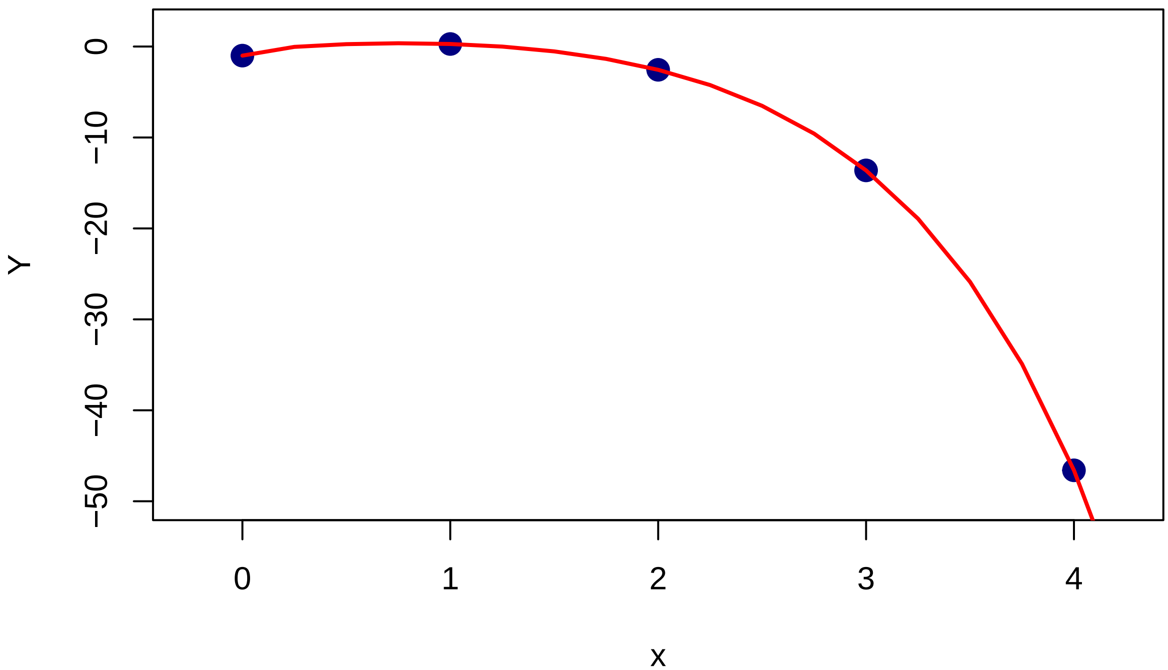
We can plot the curve corresponding to the least squares estimators using the following code.

```r
# Plot observations.
plot(x = 0:4, xlab = "x",
     y = c(-1, 0.28, -2.56, -13.62, -46.60), ylab = "Y",
     xlim = c(-1/4, 4 + 1/4),
     ylim = c(-50, 2), col = "navy",
     pch = 19, cex = 1.5)

# Generate sequence of independent variables.
xs <- seq(from = 0, to = 4.25, by = 0.25)

# Predict points on curve using least-squares model
ys <- hBetaN[1] + hBetaN[2]*xs + hBetaN[3]*sqrt(xs) + hBetaN[4]*exp(xs)

# Plot least-squares curve
lines(xs, ys, col = "red", lwd = 2)
```



0
−10
−20
−30
−40
−50
Y
0
1
2
3
4
x