1. Introduction: Linear Regression - Geometric interpretation

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Contents

1 Intro

1.1 Data

Dataset with 3 observation (X,Y):

```r
library(tidyverse)
data <- data.frame(x=1:3,y=c(1,2,2))
data
```

```
##   x y
## 1 1 1
## 2 2 2
## 3 3 2
```

1.2 Model

$$y_i = \beta_0 + \beta_1 x + \epsilon_i$$

If we write the model for each observation:

$$\begin{array}{ccc} 1 & = & \beta_0 + \beta_1 1 + \epsilon_1 \\ 2 & = & \beta_0 + \beta_1 2 + \epsilon_2 \\ 2 & = & \beta_0 + \beta_1 2 + \epsilon_3 \end{array}$$

We can also write this in matrix form

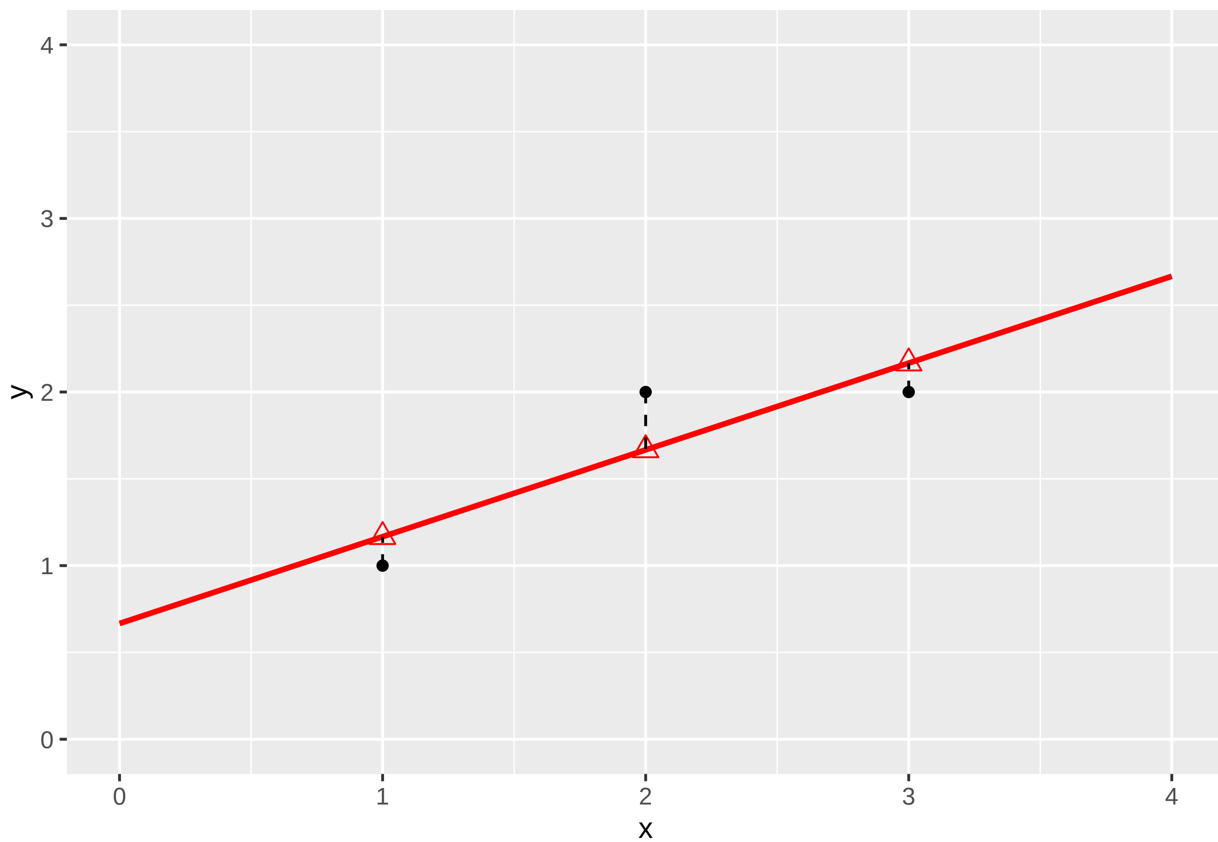
$$\mathbf{Y} = \mathbf{X}\beta + \epsilon$$

with

$$\mathbf{Y} = \left[\begin{array}{c} 1 \\ 2 \\ 2 \end{array}\right], \quad \mathbf{X} = \left[\begin{array}{cc} 1 & 1 \\ 1 & 2 \\ 1 & 3 \end{array}\right], \quad \beta = \left[\begin{array}{c} \beta_0 \\ \beta_1 \end{array}\right] \quad \text{and} \quad \epsilon = \left[\begin{array}{c} \epsilon_1 \\ \epsilon_2 \\ \epsilon_3 \end{array}\right]$$

```
lm1 <- lm(y~x,data)
data$yhat <- lm1$fitted

data %>%
  ggplot(aes(x,y)) +
  geom_point() +
  ylim(0,4) +
  xlim(0,4) +
  stat_smooth(method = "lm", color = "red", fullrange = TRUE) +
  geom_point(aes(x=x, y =yhat), pch = 2, size = 3, color = "red") +
  geom_segment(data = data, aes(x = x, xend = x, y = y, yend = yhat), lty = 2 )
```

```
## `geom_smooth()` using formula 'y ~ x'

## Warning in max(ids, na.rm = TRUE): no non-missing arguments to max; returning
## -Inf
```



2 Least Squares (LS)

- Minimize the residual sum of squares

$$
\begin{aligned}
RSS(\beta) &= \sum_{i=1}^{n} e_i^2 \\
&= \sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} x_{ij}\beta_j \right)^2
\end{aligned}
$$

- or in matrix notation

$$
\begin{aligned}
RSS(\beta) &= (\mathbf{Y} - \mathbf{X}\ )^T(\mathbf{Y} - \mathbf{X}\ ) \\
&= \|\mathbf{Y} - \mathbf{X}\ \|_2^2
\end{aligned}
$$

  with the L_2-norm of a p-dim. vector v $\|\mathbf{v}\|_2 = \sqrt{v_1^2 + ... + v_p^2} \to \hat{\beta} = \text{argmin}_\beta \|\mathbf{Y} - \mathbf{X}\ \|^2$

2.1 Minimize RSS

$$
\begin{aligned}
\frac{\partial RSS}{\partial \beta} &= \mathbf{0} \\
\frac{(\mathbf{Y}-\mathbf{X}\ )^T(\mathbf{Y}-\mathbf{X}\beta)}{\partial \beta} &= \mathbf{0} \\
-2\mathbf{X}^T(\mathbf{Y}-\mathbf{X}\beta) &= \mathbf{0} \\
\mathbf{X}^T\mathbf{X} &= \mathbf{X}^T\mathbf{Y} \\
\hat{\beta} &= (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Y}
\end{aligned}
$$

$$\hat{\beta} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Y}$$

2.2 Fitted values:

$$
\begin{aligned}
\hat{\mathbf{Y}} &= \mathbf{X}\hat{\beta} \\
&= \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Y}
\end{aligned}
$$

3 Geometric interpretation of Linear regression

There is also another picture to interpret linear regression!

Linear regression can also be seen as a projection!

Fitted values:

$$
\begin{aligned}
\hat{\mathbf{Y}} &= \mathbf{X}\hat{\beta} \\
&= \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Y} \\
&= \mathbf{HY}
\end{aligned}
$$

with $\mathbf{H}$ the projection matrix also referred to as the hat matrix.

```r
X <- model.matrix(~x,data)
X
```

```
##   (Intercept) x
## 1           1 1
## 2           1 2
## 3           1 3
## attr(,"assign")
## [1] 0 1
```

```r
XtX <- t(X)%*%X
XtX
```

```
##             (Intercept)  x
## (Intercept)           3  6
## x                     6 14
```

```
XtXinv <- solve(t(X)%*%X)
XtXinv
```

```
##             (Intercept)    x
## (Intercept)    2.333333 -1.0
## x             -1.000000  0.5
```

```
H <- X %*% XtXinv %*% t(X)
H
```

```
##            1         2          3
## 1  0.8333333 0.3333333 -0.1666667
## 2  0.3333333 0.3333333  0.3333333
## 3 -0.1666667 0.3333333  0.8333333
```

```
Y <- data$y
Yhat <- H%*%Y
Yhat
```

```
##       [,1]
## 1 1.166667
## 2 1.666667
## 3 2.166667
```

3.1 What do these projections mean geometrically?

The other picture to linear regression is to consider X_0, X_1 and Y as vectors in the space of the data $\mathbb{R}^n$, here $\mathbb{R}^3$ because we have three data points.

```
originRn <- data.frame(X1=0,X2=0,X3=0)
data$x0 <- 1
dataRn <- data.frame(t(data))

library(plotly)

p1 <- plot_ly(
    originRn,
    x = ~ X1,
    y = ~ X2,
    z= ~ X3) %>%
  add_markers(type="scatter3d") %>%
  layout(
    scene = list(
      aspectmode="cube",
      xaxis = list(range=c(-4,4)), yaxis = list(range=c(-4,4)), zaxis = list(range=c(-4,4))
      )
    )
p1 <- p1 %>%
  add_trace(
    x = c(0,1),
    y = c(0,0),
```

```
    z = c(0,0),
    mode = "lines",
    line = list(width = 5, color = "grey"),
    type="scatter3d") %>%
  add_trace(
    x = c(0,0),
    y = c(0,1),
    z = c(0,0),
    mode = "lines",
    line = list(width = 5, color = "grey"),
    type="scatter3d") %>%
  add_trace(
    x = c(0,0),
    y = c(0,0),
    z = c(0,1),
    mode = "lines",
    line = list(width = 5, color = "grey"),
    type="scatter3d") %>%
  add_trace(
    x = c(0,1),
    y = c(0,1),
    z = c(0,1),
    mode = "lines",
    line = list(width = 5, color = "black"),
    type="scatter3d") %>%
    add_trace(
    x = c(0,1),
    y = c(0,2),
    z = c(0,3),
    mode = "lines",
    line = list(width = 5, color = "black"),
    type="scatter3d")
```

```
p2 <- p1 %>%
  add_trace(
    x = c(0,Y[1]),
    y = c(0,Y[2]),
    z = c(0,Y[3]),
    mode = "lines",
    line = list(width = 5, color = "red"),
    type="scatter3d") %>%
  add_trace(
    x = c(0,Yhat[1]),
    y = c(0,Yhat[2]),
    z = c(0,Yhat[3]),
    mode = "lines",
    line = list(width = 5, color = "red"),
    type="scatter3d") %>% add_trace(
    x = c(Y[1],Yhat[1]),
    y = c(Y[2],Yhat[2]),
    z = c(Y[3],Yhat[3]),
    mode = "lines",
    line = list(width = 5, color = "red", dash="dash"),
```

```
    type="scatter3d")
p2
```

3.1.1 How does this projection work?

$$
\begin{aligned}
\hat{\mathbf{Y}} &= \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Y} \\
&= \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1/2}(\mathbf{X}^T\mathbf{X})^{-1/2}\mathbf{X}^T\mathbf{Y} \\
&= \mathbf{U}\mathbf{U}^T\mathbf{Y}
\end{aligned}
$$

- $\mathbf{U}$ is a new orthonormal basis in $\mathbb{R}^2$, a subspace of $\mathbb{R}^3$
- The space spanned by U and X is the column space of X, e.g. it contains all possible linear combinantions of X. $\mathbf{U}^t\mathbf{Y}$ is the projection of Y on this new orthonormal basis

```
eigenXtX <- eigen(XtX)
XtXinvSqrt <- eigenXtX$vectors %*%diag(1/eigenXtX$values^.5)%*%t(eigenXtX$vectors)
U <- X %*% XtXinvSqrt

p3 <- p1 %>%
  add_trace(
    x = c(0,U[1,1]),
    y = c(0,U[2,1]),
    z = c(0,U[3,1]),
    mode = "lines",
    line = list(width = 5, color = "blue"),
    type="scatter3d") %>%
  add_trace(
    x = c(0,U[1,2]),
    y = c(0,U[2,2]),
    z = c(0,U[3,2]),
    mode = "lines",
    line = list(width = 5, color = "blue"),
    type="scatter3d")

p3
```

- $\mathbf{U}^T\mathbf{Y}$ is the projection of $\mathbf{Y}$ in the space spanned by $\mathbf{U}$.
- Indeed $\mathbf{U}_1^T\mathbf{Y}$

```
p4 <- p3 %>%
  add_trace(
    x = c(0,Y[1]),
    y = c(0,Y[2]),
    z = c(0,Y[3]),
    mode = "lines",
    line = list(width = 5, color = "red"),
    type="scatter3d") %>%
  add_trace(
    x = c(0,U[1,1]*(U[,1]%*%Y)),
    y = c(0,U[2,1]*(U[,1]%*%Y)),
    z = c(0,U[3,1]*(U[,1]%*%Y)),
```

```
    mode = "lines",
    line = list(width = 5, color = "red",dash="dash"),
    type="scatter3d") %>% add_trace(
    x = c(Y[1],U[1,1]*(U[,1]%*%Y)),
    y = c(Y[2],U[2,1]*(U[,1]%*%Y)),
    z = c(Y[3],U[3,1]*(U[,1]%*%Y)),
    mode = "lines",
    line = list(width = 5, color = "red", dash="dash"),
    type="scatter3d")
p4
```

- and $\mathbf{U}_2^T\mathbf{Y}$

```
p5 <- p4 %>%
  add_trace(
    x = c(0,Y[1]),
    y = c(0,Y[2]),
    z = c(0,Y[3]),
    mode = "lines",
    line = list(width = 5, color = "red"),
    type="scatter3d") %>%
  add_trace(
    x = c(0,U[1,2]*(U[,2]%*%Y)),
    y = c(0,U[2,2]*(U[,2]%*%Y)),
    z = c(0,U[3,2]*(U[,2]%*%Y)),
    mode = "lines",
    line = list(width = 5, color = "red",dash="dash"),
    type="scatter3d") %>% add_trace(
    x = c(Y[1],U[1,2]*(U[,2]%*%Y)),
    y = c(Y[2],U[2,2]*(U[,2]%*%Y)),
    z = c(Y[3],U[3,2]*(U[,2]%*%Y)),
    mode = "lines",
    line = list(width = 5, color = "red", dash="dash"),
    type="scatter3d")
p5
```

```
p6 <- p5 %>%
  add_trace(
    x = c(0,Yhat[1]),
    y = c(0,Yhat[2]),
    z = c(0,Yhat[3]),
    mode = "lines",
    line = list(width = 5, color = "red"),
    type="scatter3d") %>%
  add_trace(
    x = c(Y[1],Yhat[1]),
    y = c(Y[2],Yhat[2]),
    z = c(Y[3],Yhat[3]),
    mode = "lines",
    line = list(width = 5, color = "red", dash="dash"),
    type="scatter3d") %>%
  add_trace(
    x = c(U[1,1]*(U[,1]%*%Y),Yhat[1]),
```

```
    y = c(U[2,1]*(U[,1]%*%Y),Yhat[2]),
    z = c(U[3,1]*(U[,1]%*%Y),Yhat[3]),
    mode = "lines",
    line = list(width = 5, color = "red", dash="dash"),
    type="scatter3d")  %>%
  add_trace(
    x = c(U[1,2]*(U[,2]%*%Y),Yhat[1]),
    y = c(U[2,2]*(U[,2]%*%Y),Yhat[2]),
    z = c(U[3,2]*(U[,2]%*%Y),Yhat[3]),
    mode = "lines",
    line = list(width = 5, color = "red", dash="dash"),
    type="scatter3d")
p6
```

3.2 The Error vector

Note, that it is also clear from the equation in the derivation of the least squares solution that the residual is orthogonal on the column space:

$$-2\mathbf{X}^T(\mathbf{Y}-\mathbf{X}\beta)=0$$

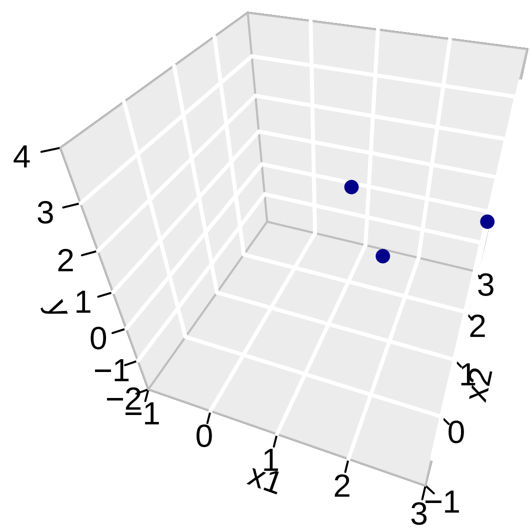
4 Curse of dimensionality?

- Imagine what happens when p approaches n $p=n$ or becomes much larger than p » n!!!
- Suppose that we add a predictor $\mathbf{X}_2=[2,0,1]^T$?

$$\mathbf{Y}=\left[\begin{array}{c}1\\2\\2\end{array}\right],\quad \mathbf{X}=\left[\begin{array}{ccc}1&1&2\\1&2&0\\1&3&1\end{array}\right],\quad \beta=\left[\begin{array}{c}\beta_0\\\beta_1\\\beta_2\end{array}\right]\quad \text{and}\quad \epsilon=\left[\begin{array}{c}\epsilon_1\\\epsilon_2\\\epsilon_3\end{array}\right]$$

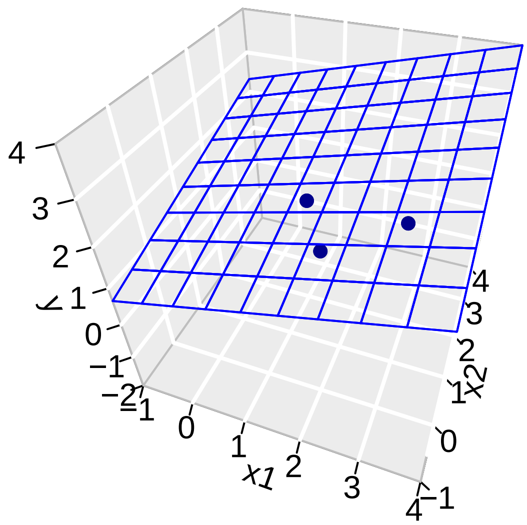
```
data$x2 <- c(2,0,1)
fit <- lm(y~x+x2,data)
# predict values on regular xy grid
x1pred <- seq(-1, 4, length.out = 10)
x2pred <- seq(-1, 4, length.out = 10)
xy <- expand.grid(x = x1pred,
x2 = x2pred)
ypred <- matrix (nrow = 30, ncol = 30,
data = predict(fit, newdata = data.frame(xy)))

library(plot3D)


# fitted points for droplines to surface
th=20
ph=5
scatter3D(data$x,
  data$x2,
  Y,
```

```
  pch = 16,
  col="darkblue",
  cex = 1,
  theta = th,
  ticktype = "detailed",
  xlab = "x1",
  ylab = "x2",
  zlab = "y",
  colvar=FALSE,
  bty = "g",
  xlim=c(-1,3),
  ylim=c(-1,3),
  zlim=c(-2,4))
```




```
z.pred3D <- outer(
  x1pred,
  x2pred,
  function(x1,x2)
  {
    fit$coef[1] + fit$coef[2]*x1+fit$coef[2]*x2
  })

x.pred3D <- outer(
  x1pred,
  x2pred,
```

```
  function(x,y) x)

y.pred3D <- outer(
  x1pred,
  x2pred,
  function(x,y) y)

scatter3D(data$x,
  data$x2,
  data$y,
  pch = 16,
  col="darkblue",
  cex = 1,
  theta = th,
  ticktype = "detailed",
  xlab = "x1",
  ylab = "x2",
  zlab = "y",
  colvar=FALSE,
  bty = "g",
  xlim=c(-1,4),
  ylim=c(-1,4),
  zlim=c(-2,4))

surf3D(
  x.pred3D,
  y.pred3D,
  z.pred3D,
  col="blue",
  facets=NA,
  add=TRUE)
```



Note, that the linear regression is now a plane.

However, we obtain a perfect fit and all the data points are falling in the plane!

This is obvious if we look at the column space of X!

```
X <- cbind(X,c(2,0,1))
XtX <- t(X)%*%X
eigenXtX <- eigen(XtX)
XtXinvSqrt <- eigenXtX$vectors %*%diag(1/eigenXtX$values^.5)%*%t(eigenXtX$vectors)
U <- X %*% XtXinvSqrt

p7 <- p1 %>%
  add_trace(
    x = c(0,2),
    y = c(0,0),
    z = c(0,1),
    mode = "lines",
    line = list(width = 5, color = "darkgreen"),
    type="scatter3d")
p7
```

```
p8 <- p7 %>%
  add_trace(
    x = c(0,U[1,1]),
    y = c(0,U[2,1]),
    z = c(0,U[3,1]),
```

```
    mode = "lines",
    line = list(width = 5, color = "blue"),
    type="scatter3d") %>%
  add_trace(
    x = c(0,U[1,2]),
    y = c(0,U[2,2]),
    z = c(0,U[3,2]),
    mode = "lines",
    line = list(width = 5, color = "blue"),
    type="scatter3d") %>%
  add_trace(
    x = c(0,U[1,3]),
    y = c(0,U[2,3]),
    z = c(0,U[3,3]),
    mode = "lines",
    line = list(width = 5, color = "blue"),
    type="scatter3d")

p8
```

- The column space now spans the entire $\mathbb{R}^3$!
- With the intercept and the two predictors we can thus fit every dataset that only has 3 observations for the predictors and the response.
- So the model can no longer be used to generalise the patterns seen in the data towards the population (new observations).
- Problem of overfitting!!!
- If $p >> n$ then the problem gets even worse! Then there is even no longer a unique solution to the least squares problem…