Least squares estimation of regression lines

Regression via least squares

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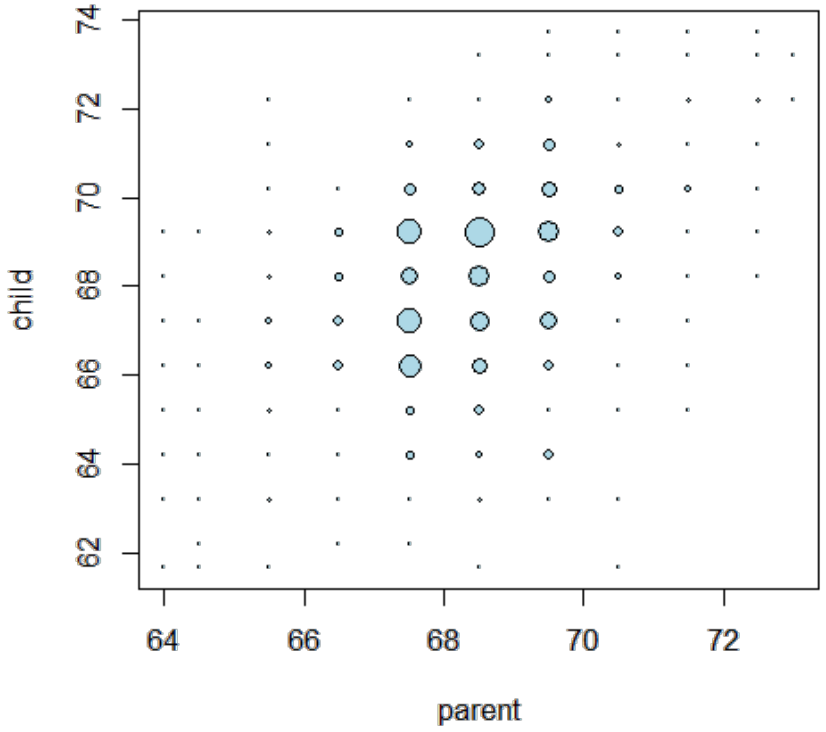
General least squares for linear equations

Consider again the parent and child height data from Galton



Fitting the best line

- Let Y_i be the i^{th} child's height and X_i be the i^{th} (average over the pair of) parents' heights.
- Consider finding the best line
  - Child's Height = β_0 + Parent's Height β_1
- Use least squares

$$\sum_{i=1}^{n} \{Y_i - (\beta_0 + \beta_1 X_i)\}^2$$

- How do we do it?

Let's solve this problem generally

- Let $\mu_i = \beta_0 + \beta_1 X_i$ and our estimates be $\hat{\mu}_i = \hat{\beta}_0 + \hat{\beta}_1 X_i$.
- We want to minimize

$$\dagger \sum_{i=1}^{n} (Y_i - \mu_i)^2 = \sum_{i=1}^{n} (Y_i - \hat{\mu}_i)^2 + 2 \sum_{i=1}^{n} (Y_i - \hat{\mu}_i)(\hat{\mu}_i - \mu_i) + \sum_{i=1}^{n} (\hat{\mu}_i - \mu_i)^2$$

- Suppose that

$$\sum_{i=1}^{n} (Y_i - \hat{\mu}_i)(\hat{\mu}_i - \mu_i) = 0$$

then

$$\dagger = \sum_{i=1}^{n} (Y_i - \hat{\mu}_i)^2 + \sum_{i=1}^{n} (\hat{\mu}_i - \mu_i)^2 \geq \sum_{i=1}^{n} (Y_i - \hat{\mu}_i)^2$$

Mean only regression

- So we know that if:

$$\sum_{i=1}^{n}(Y_i - \hat{\mu}_i)(\hat{\mu}_i - \mu_i) = 0$$

where $\mu_i = \beta_0 + \beta_1 X_i$ and $\hat{\mu}_i = \hat{\beta}_0 + \hat{\beta}_1 X_i$ then the line

$$Y = \hat{\beta}_0 + \hat{\beta}_1 X$$

is the least squares line.

- Consider forcing $\beta_1 = 0$ and thus $\hat{\beta}_1 = 0$; that is, only considering horizontal lines
- The solution works out to be

$$\hat{\beta}_0 = \bar{Y}.$$

Let's show it

$$\sum_{i=1}^{n}(Y_i - \hat{\mu}_i)(\hat{\mu}_i - \mu_i) = \sum_{i=1}^{n}(Y_i - \hat{\beta}_0)(\hat{\beta}_0 - \beta_0)$$

$$= (\hat{\beta}_0 - \beta_0)\sum_{i=1}^{n}(Y_i - \hat{\beta}_0)$$

Thus, this will equal 0 if $\sum_{i=1}^{n}(Y_i - \hat{\beta}_0) = n\bar{Y} - n\hat{\beta}_0 = 0$

Thus $\hat{\beta}_0 = \bar{Y}$.

Regression through the origin

- Recall that if:

$$\sum_{i=1}^{n}(Y_i - \hat{\mu}_i)(\hat{\mu}_i - \mu_i) = 0$$

where $\mu_i = \beta_0 + \beta_1 X_i$ and $\hat{\mu}_i = \hat{\beta}_0 + \hat{\beta}_1 X_i$ then the line

$$Y = \hat{\beta}_0 + \hat{\beta}_1 X$$

is the least squares line.

- Consider forcing $\beta_0 = 0$ and thus $\hat{\beta}_0 = 0$; that is, only considering lines through the origin
- The solution works out to be

$$\hat{\beta}_1 = \frac{\sum_{i=1^n} Y_i X_i}{\sum_{i=1}^{n} X_i^2}.$$

Let's show it

$$\sum_{i=1}^{n}(Y_i - \hat{\mu}_i)(\hat{\mu}_i - \mu_i) = \sum_{i=1}^{n}(Y_i - \hat{\beta}_1 X_i)(\hat{\beta}_1 X_i - \beta_1 X_i)$$

$$= (\hat{\beta}_1 - \beta_1)\sum_{i=1}^{n}(Y_i X_i - \hat{\beta}_1 X_i^2)$$

Thus, this will equal 0 if $\sum_{i=1}^{n}(Y_i X_i - \hat{\beta}_1 X_i^2) = \sum_{i=1}^{n} Y_i X_i - \hat{\beta}_1 \sum_{i=1}^{n} X_i^2 = 0$

Thus

$$\hat{\beta}_1 = \frac{\sum_{i=1^n} Y_i X_i}{\sum_{i=1}^{n} X_i^2}.$$

Recapping what we know

- If we define $\mu_i = \beta_0$ then $\hat{\beta}_0 = \bar{Y}$.
  - If we only look at horizontal lines, the least squares estimate of the intercept of that line is the average of the outcomes.
- If we define $\mu_i = X_i\beta_1$ then $\hat{\beta}_1 = \frac{\sum_{i=1}^{n} Y_i X_i}{\sum_{i=1}^{n} X_i^2}$
  - If we only look at lines through the origin, we get the estimated slope is the cross product of the X and Ys divided by the cross product of the Xs with themselves.
- What about when $\mu_i = \beta_0 + \beta_1 X_i$? That is, we don't want to restrict ourselves to horizontal lines or lines through the origin.

Let's figure it out

$$\sum_{i=1}^{n}(Y_i - \hat{\mu}_i)(\hat{\mu}_i - \mu_i) = \sum_{i=1}^{n}(Y_i - \hat{\beta}_0 - \hat{\beta}_1 X_i)(\hat{\beta}_0 + \hat{\beta}_1 X_i - \beta_0 - \beta_1 X_i)$$

$$= (\hat{\beta}_0 - \beta_0)\sum_{i=1}^{n}(Y_i - \hat{\beta}_0 - \hat{\beta}_1 X_i) + (\beta_1 - \beta_1)\sum_{i=1}^{n}(Y_i - \hat{\beta}_0 - \hat{\beta}_1 X_i)X_i$$

Note that

$$0 = \sum_{i=1}^{n}(Y_i - \hat{\beta}_0 - \hat{\beta}_1 X_i) = n\bar{Y} - n\hat{\beta}_0 - n\hat{\beta}_1\bar{X} \text{ implies that } \hat{\beta}_0 = \bar{Y} - \hat{\beta}_1\bar{X}$$

Then

$$\sum_{i=1}^{n}(Y_i - \hat{\beta}_0 - \hat{\beta}_1 X_i)X_i = \sum_{i=1}^{n}(Y_i - \bar{Y} + \hat{\beta}_1\bar{X} - \hat{\beta}_1 X_i)X_i$$

Continued

$$= \sum_{i=1}^{n} \{(Y_i - \bar{Y}) - \hat{\beta}_1(X_i - \bar{X})\}X_i$$

And thus

$$\sum_{i=1}^{n}(Y_i - \bar{Y})X_i - \hat{\beta}_1 \sum_{i=1}^{n}(X_i - \bar{X})X_i = 0.$$

So we arrive at

$$\hat{\beta}_1 = \frac{\sum_{i=1}^{n}\{(Y_i - \bar{Y})X_i}{\sum_{i=1}^{n}(X_i - \bar{X})X_i} = \frac{\sum_{i=1}^{n}(Y_i - \bar{Y})(X_i - \bar{X})}{\sum_{i=1}^{n}(X_i - \bar{X})(X_i - \bar{X})} = \mathrm{Cor}(Y, X)\,\frac{\mathrm{Sd}(Y)}{\mathrm{Sd}(X)}\,.$$

And recall

$$\hat{\beta}_0 = \bar{Y} - \hat{\beta}_1\bar{X}.$$

Consequences

- The least squares model fit to the line $Y = \beta_0 + \beta_1 X$ through the data pairs (X_i, Y_i) with Y_i as the outcome obtains the line $Y = \hat{\beta}_0 + \hat{\beta}_1 X$ where

$$\hat{\beta}_1 = \text{Cor}(Y, X)\frac{\text{Sd}(Y)}{\text{Sd}(X)} \quad \hat{\beta}_0 = \bar{Y} - \hat{\beta}_1 \bar{X}$$

- $\hat{\beta}_1$ has the units of Y/X, $\hat{\beta}_0$ has the units of Y.
- The line passes through the point $(\bar{X}, \bar{Y})$
- The slope of the regression line with X as the outcome and Y as the predictor is $\text{Cor}(Y, X)\text{Sd}(X)/\text{Sd}(Y)$.
- The slope is the same one you would get if you centered the data, $(X_i - \bar{X}, Y_i - \bar{Y})$, and did regression through the origin.
- If you normalized the data, $\{\frac{X_i - \bar{X}}{\text{Sd}(X)}, \frac{Y_i - \bar{Y}}{\text{Sd}(Y)}\}$, the slope is $\text{Cor}(Y, X)$.

Revisiting Galton's data

Double check our calculations using R

```
y <- galton$child
x <- galton$parent
beta1 <- cor(y, x) *  sd(y) / sd(x)
beta0 <- mean(y) - beta1 * mean(x)
rbind(c(beta0, beta1), coef(lm(y ~ x)))
```

```
     (Intercept)      x
[1,]       23.94 0.6463
[2,]       23.94 0.6463
```

Revisiting Galton's data

Reversing the outcome/predictor relationship

```
beta1 <- cor(y, x) *  sd(x) / sd(y)
beta0 <- mean(x) - beta1 * mean(y)
rbind(c(beta0, beta1), coef(lm(x ~ y)))
```

```
     (Intercept)      y
[1,]       46.14 0.3256
[2,]       46.14 0.3256
```

Revisiting Galton's data

Regression through the origin yields an equivalent slope if you center the data first

```
yc <- y - mean(y)
xc <- x - mean(x)
beta1 <- sum(yc * xc) / sum(xc ^ 2)
c(beta1, coef(lm(y ~ x))[2])
```

```
           x
0.6463 0.6463
```

Revisiting Galton's data

Normalizing variables results in the slope being the correlation

```
yn <- (y - mean(y))/sd(y)
xn <- (x - mean(x))/sd(x)
c(cor(y, x), cor(yn, xn), coef(lm(yn ~ xn))[2])
```

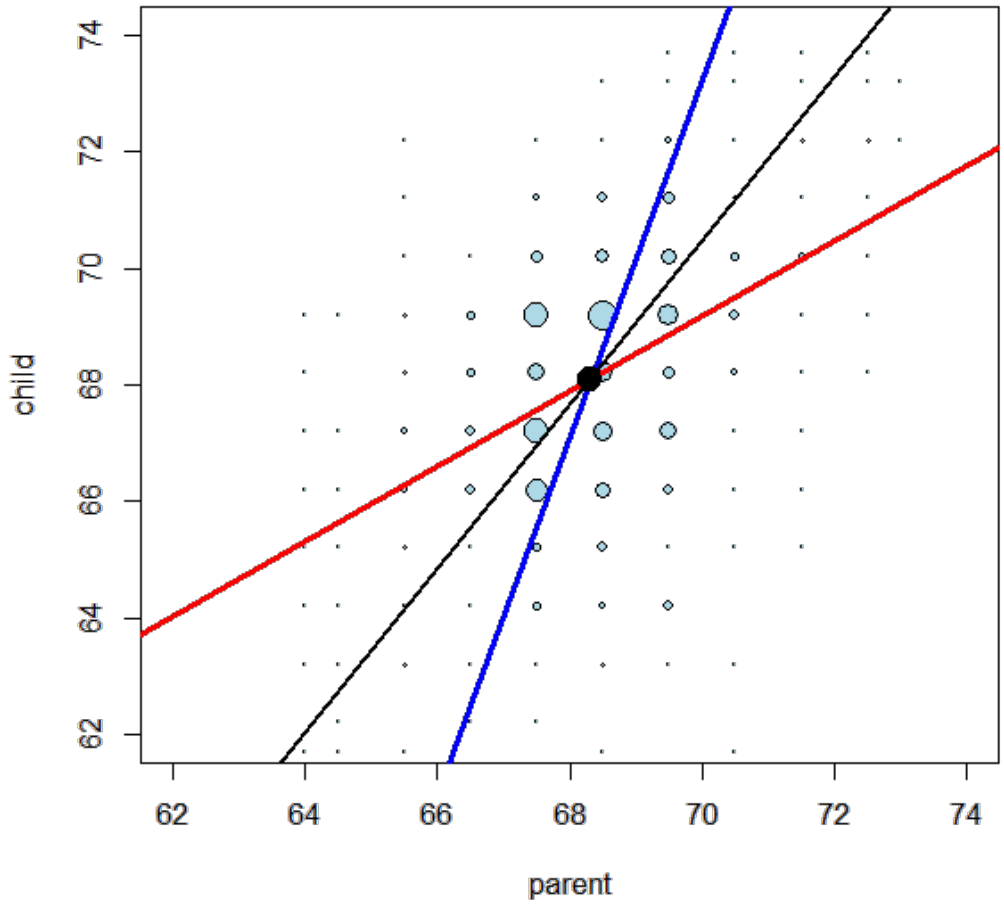
```
                 xn
0.4588 0.4588 0.4588
```

Plotting the fit

- Size of points are frequencies at that X, Y combination.
- For the red lie the child is outcome.
- For the blue, the parent is the outcome (accounting for the fact that the response is plotted on the horizontal axis).
- Black line assumes $\mathrm{Cor}(\mathrm{Y}, \mathrm{X}) = 1$ (slope is $\mathrm{Sd}(\mathrm{Y})/\mathrm{Sd}(\mathrm{x})$).
- Big black dot is $(\bar{\mathrm{X}}, \bar{\mathrm{Y}})$.

The code to add the lines

```
abline(mean(y) - mean(x) * cor(y, x) * sd(y) / sd(x),
  sd(y) / sd(x) * cor(y, x),
  lwd = 3, col = "red")
abline(mean(y) - mean(x) * sd(y) / sd(x) / cor(y, x),
  sd(y) cor(y, x) / sd(x),
  lwd = 3, col = "blue")
abline(mean(y) - mean(x) * sd(y) / sd(x),
  sd(y) / sd(x),
  lwd = 2)
points(mean(x), mean(y), cex = 2, pch = 19)
```


child
parent
62
64
66
68
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