Least squares estimation of regression lines

Regression via least squares

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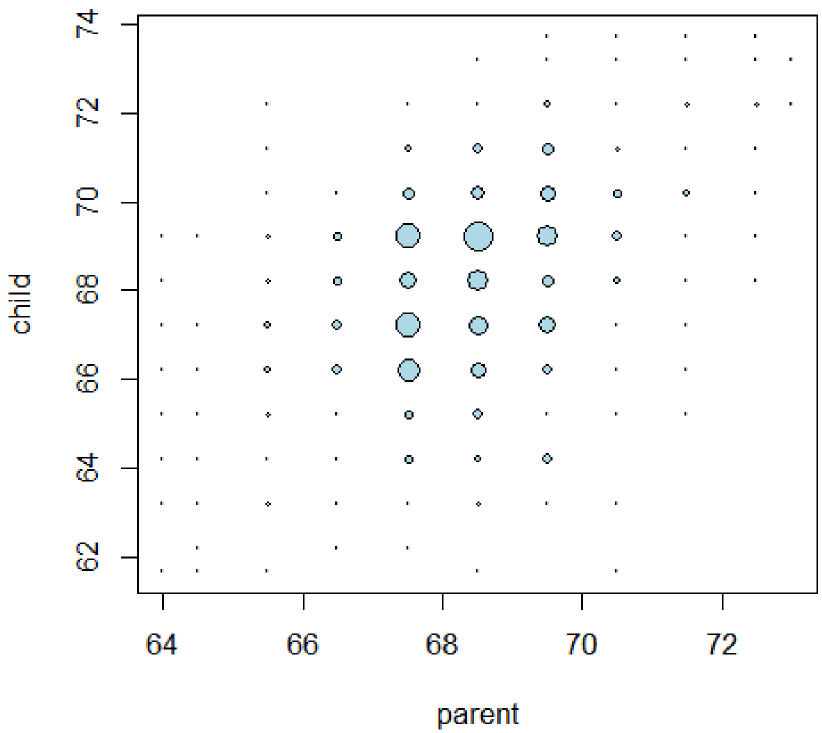
General least squares for linear equations

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

observed

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

predicted

see Ng in
Machine Learning!

- How do we do it?

Let's solve this problem generally

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

mu_i^ und beta_0/1^ sind unsere Voraussagen.
mu_i resp beta_0/1 sind irgendwelche /anderen/ Voraussagen.

- We want to minimize

Add and extract my_i^ (wie beim Beweis, dass Min der Summe der squared Dist. = mean),
then expand the square:

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

1.Summe:
Diff zw. Y_i und originalen Voraussage mu_i^

2. Summe:
Diff zw originalen Voraussage und neuen, geaenderten Voraussage

- Suppose that

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

then

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

Diese Summe ist immer > 0

Also fuer /irgendein/ mu_i ist die Summe der quadrierten Distanzen groesser als wenn man das vorhergesagte mu nimmt! HX

Sofern die mittlere Summe == 0! Siehe unten..

=> gleicher Trick wie beim Beweis, dass Min der Summe der squared Dist. = mean)

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

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

-> die beste Voraussage ist das mean, dann.

(haben wir schon frueher bewiesen, und wie die naechste Slide nochmal beweist)

Let's show it

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

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

^ siehe frueher)

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
  not beta1, but beta0 ist jetzt = 0, also ^
- The solution works out to be

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

$\dfrac{< Y, X >}{< X, X >}$ (inner product)

Let's show it

```
mu_i  = beta1 * x_i
mu_i^ = beta1^ * x_i
```

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

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

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

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

```
Bei /diesem/ beta1^ wird der erste Term
oben = 0, und /dann/ ist die Gerade

Y = beta0^ + beta1^ * X

die Gerade der kleinsten Quadrate!
```

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 $\hat{\beta}_1 = \frac{\sum_{i=1^n} Y_i X_i}{\sum_{i=1}^n X_i^2}$ =sum of squares of X_i
  - 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

mu_i = beta0 + beta1 * x_i
mu_i^ = beta0^ + beta1^ * x_i

-> einsetzen:

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

das soll 0 werden

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

falls dieser Term 0 waere …

… und dieser Term auch 0 waere, dann haetten wir, was wir wollen!

Note that

Wir haben also 2 Gleichungen und zwei Unbekannte!

einsetzen

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

einfach nach beta0^ aufloesen

Then

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

das koennen wir jetzt 0 setzen

Continued

$$= \sum_{i=1}^{n} \{\underbrace{(Y_i - \bar{Y})}_{\text{centered Ys}} - \hat{\beta}_1 \underbrace{(X_i - \bar{X})}_{\text{centered Xs}}\} X_i$$

And thus

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

nach beta1^ aufloesen:

So we arrive at

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

And recall

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

Das stellt sicher, dass die Regressionslinie
immer durch den Punkt (X_, Y_) geht!

sum(y_i - y_) x_ = x_ sum(y_i - y_) =

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

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

slope intercept

- $\hat{\beta}_1$ has the units of Y/X, $\hat{\beta}_0$ has the units of Y. weil Cor(Y,X) hat keine Einheit, also bleibt Einheit Y/Einheit X, was Sinn macht fuer eine Steigung
- 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 $Cor(Y, X) Sd(X)/Sd(Y)$. Inverse Funktion
- 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, $\{\frac{X_i - \bar{X}}{Sd(X)}, \frac{Y_i - \bar{Y}}{Sd(Y)}\}$, the slope is $Cor(Y, X)$.

weil dann die SDs = 1 eins, also bleibt die Korrelation.

Revisiting Galton's data

Double check our calculations using R

```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)))    einfach umgekehrt
```

```
     (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])
```

centering

```
            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])
```

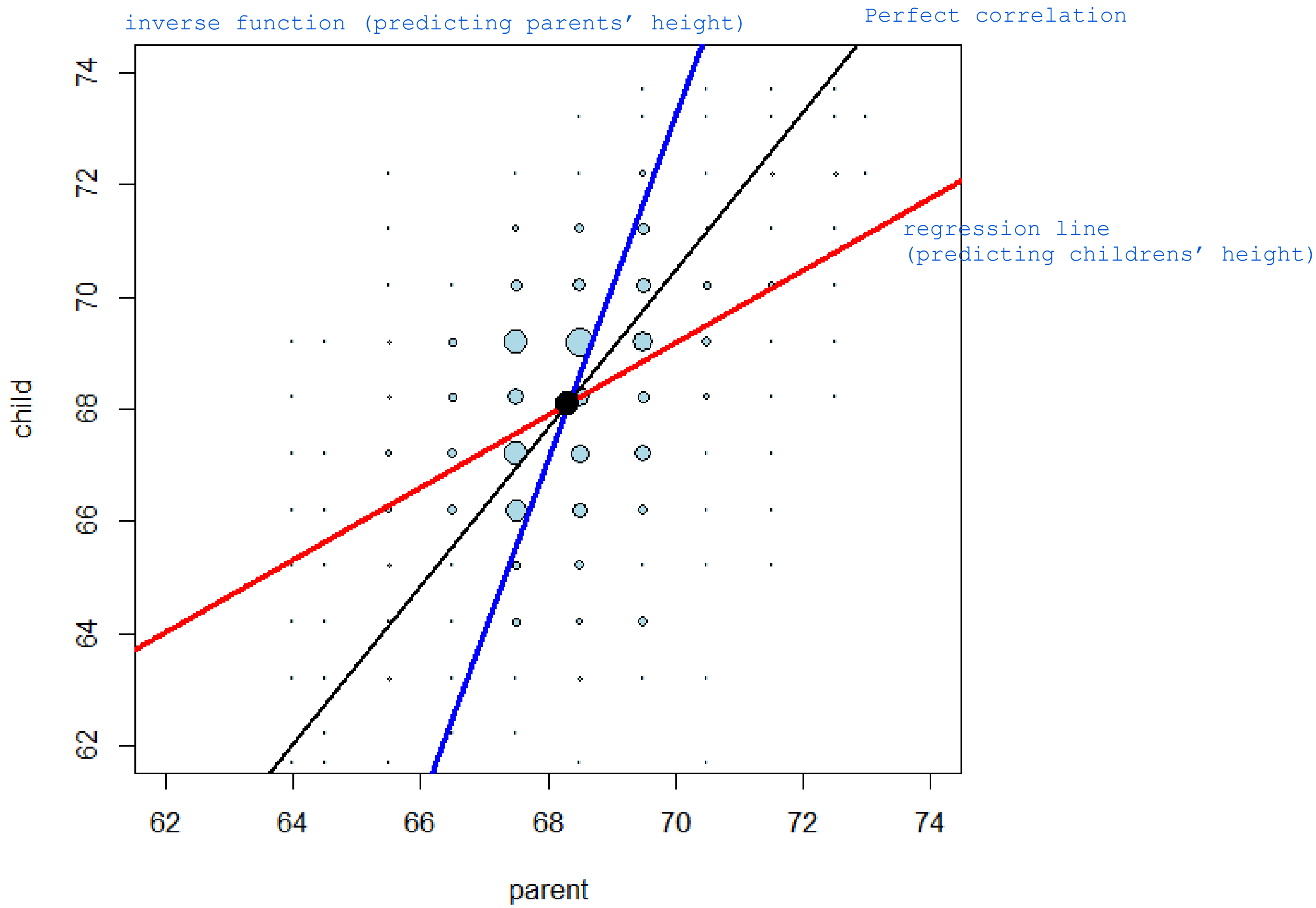
```
                  xn
0.4588 0.4588 0.4588
```

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 $\mathrm{Cor}(Y, X) = 1$ (slope is $\mathrm{Sd}(Y)/\mathrm{Sd}(x)$).
- Big black dot is $(\bar{X}, \bar{Y})$.

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)
```



var(data)=var(estimate)+var(residuals)