Regression and Linear Models (37252) Lecture 2 - Simple Linear Regression I

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These notes are based, in part, on earlier versions prepared by Dr Ed Lidums and Prof. James Brown.

2. Lecture outline

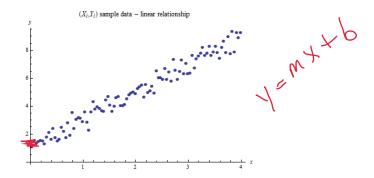
Topics:

- fitting lines to data
 - model setup
 - method of least squares
 - data transformations
- model assumptions
- model parameters and estimates
- statistical properties of estimates
 - distributions
 - T-tests
- statistical properties of model
 - prediction of $\mathbb{E}[Y|x]$
 - prediction of Y|x
- human calculator example
- R example

See Chapters 1 and 2 of Draper and Smith (1998).

2. Fitting lines to data

Consider the problem of constructing a model describing the **sample** data (X_i, Y_i) , $i \in \{1, ..., n\}$, displayed in the following scatter plot.



In this toy example, the sample data has been generated using the rule

 $Y_i = 1 + 2X_i + \epsilon_i$ with n = 100, $X_i = \frac{4}{n}i$ and $\epsilon_i \sim N(0, \frac{1}{2})$.

2. Fitting lines to data – model setup

You immediately notice a strong, although imperfect, **linear** relationship in the data and wonder whether the underlying **population** might be described by

$$Y = \beta_0 + \beta_1 x + \epsilon_2$$

which is the equation of a straight line with intercept β_0 , slope β_1 that is disturbed by some RV ϵ . This of course makes Y a random variable also.

$$\hat{Y}|x := \hat{\beta}_0 + \hat{\beta}_1 x$$

$$\approx \mathbb{E}[Y|x]$$
(2)

will be determined by the quality of the estimates $\hat{\beta}_0$ and $\hat{\beta}_1$.

There are many methods that are suitable to this situation, but the one that is most widely used is the **method of least squares**.

This is because the estimates $\hat{\beta}_0$ and $\hat{\beta}_1$ are known in **closed-form**, which means they can be calculated **exactly**.

Later in the course we will study another technique in regression ("logistic" regression) where the model parameters can only be approximated.

The method of least squares is based on the idea of finding the estimated coefficients $\hat{\beta}_0$ and $\hat{\beta}_1$ such that error in the approximation $\hat{\epsilon} := Y - \hat{Y}$ obs, -0stimuted $= Y - \hat{\beta}_0 - \hat{\beta}_1 x$

is minimised in some way.

This error term \hat{e} is an estimate of the RV

$$\epsilon = Y - \beta_0 - \beta_1 x$$

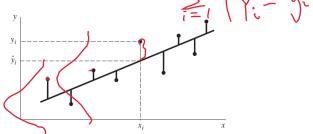
assumed in the population model underlying the sample data.

The least squares model is the model that minimises the sum squared errors over the sample data; i.e. $\gamma_i - (\beta_0 + \beta_1 + \beta_2)$

$$\min_{(\beta_0,\beta_1)} SSE(\beta_0,\beta_1) = \min_{(\beta_0,\beta_1)} \sum_{i=1}^n (Y_i - \beta_0 - \beta_1 X_i)^2$$
$$= \sum_{i=1}^n (Y_i - \hat{\beta}_0 - \hat{\beta}_1 X_i)^2.$$
(3)

¥:

The residual $\hat{\epsilon}_i$ associated with the *i*-th data point (X_i, Y_i) is the distance between the sample data value Y_i and the value \hat{Y}_i determined by the regression model line.



Regression line residual. Source: Wackerly et al. (2008) page 569

Assuming that the minimum of *SSE* exists, we can find $\hat{\beta}_0$ and $\hat{\beta}_1$ by differentiating *SSE* with respect to both β_0 and β_1 , setting the equations to zero and solving.

That is, $\hat{\beta_0}$ will be found as the value such that

$$\frac{\partial}{\partial\beta_0} SSE(\beta_0, \beta_1)|_{\beta_0 = \hat{\beta}_0} = 0$$
(4)

and $\hat{\beta_1}$ such that

$$\frac{\partial}{\partial\beta_1} SSE(\beta_0, \beta_1)|_{\beta_1 = \hat{\beta}_1} = 0.$$
(5)

The resulting regression line

$$\hat{Y}|x = \hat{\beta}_0 + \hat{\beta}_1 x$$

is the straight line that minimises total SSE associated with the sample data.

After performing the differentiation, the **least squares equations** (4) and (5) become

$$\sum_{i=1}^{n} Y_{i} - n\hat{\beta}_{0} - \hat{\beta}_{1} \sum_{i=1}^{n} X_{i} = 0$$
 (6)

$$\sum_{i=1}^{n} X_{i}Y_{i} - \hat{\beta}_{0}\sum_{i=1}^{n} X_{i} - \hat{\beta}_{1}\sum_{i=1}^{n} X_{i}^{2} = 0$$
(7)

respectively, which after solving provide the least squares coefficients

$$\hat{\beta}_1 = \frac{\sum_{i=1}^n (X_i - \overline{X})(Y_i - \overline{Y})}{\sum_{i=1}^n (X_i - \overline{X})^2} \quad \underbrace{\underbrace{Sx}}_{\underbrace{Sxx}}$$

and

Var(XI-X)

and

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

These are often re-expressed as

$$\hat{\beta}_1 = \frac{S_{XY}}{S_{XX}} \tag{8}$$

and

$$\hat{\beta}_0 = \overline{Y} - \hat{\beta}_1 \overline{X} \tag{9}$$

where

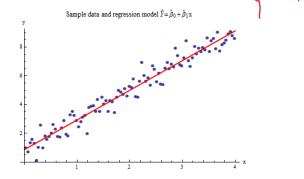
$$S_{XY} = \sum_{i=1}^{n} (X_i - \overline{X})(Y_i - \overline{Y})$$
(10)

and

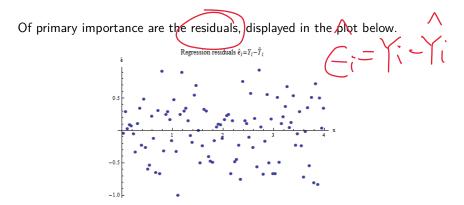
$$S_{XX} = \sum_{i=1}^{n} (X_i - \overline{X})^2.$$
(11)

The least squares problem is solved.

The following graph shows the least squares line fitted to the sample 2^{-1} data.

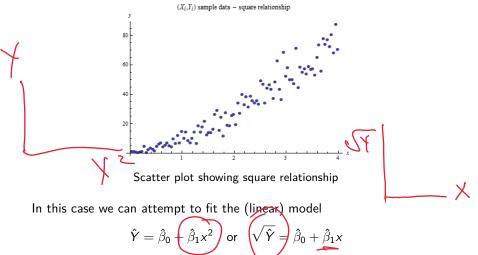


The least squares coefficients are $\hat{\beta}_0 = 1.07678$ and $\hat{\beta}_1 = 1.96832$.



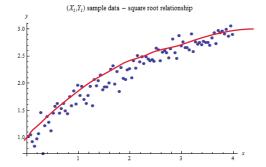
In building regression models, much of our effort will be spent analyzing the residuals for compliance with assumptions (more soon).

What if the data does not seem linear?



using the first alternative if the Y_i sample data take negative values.

Here is another example showing a square root relationship.

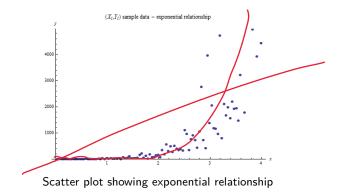


Scatter plot showing square root relationship

In this case we can attempt to fit the model $\hat{Y} = \hat{\beta}_0 + \hat{\beta}_1 \sqrt{x} \text{ or } \hat{Y}^2 = \hat{\beta}_0 + \hat{\beta}_1 x$

using the second alternative if the X_i sample data take negative values.

Another example showing an exponential relationship.

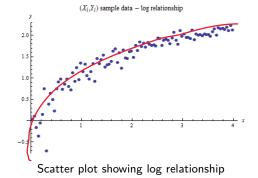


In this case we can attempt to fit the model

$$\hat{Y} = \hat{\beta}_0 + \hat{\beta}(e^{x})$$
 or $\left(\log(\hat{Y}) \neq \hat{\beta}_0 + \hat{\beta}_1 x\right)$

using the first alternative if the Y_i sample data take negative values.

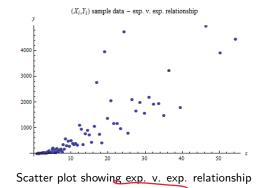
Another example showing a log relationship.



In this case we can attempt to fit the model $\hat{Y} = \hat{\beta}_0 + \hat{\beta}_1 \log x \quad \text{or} \quad e^{\hat{Y}} = \hat{\beta}_0 + \hat{\beta}_1 x$

using the second alternative if the X_i sample data take negative values.

Sometimes we need to transform both X_i and Y_i .

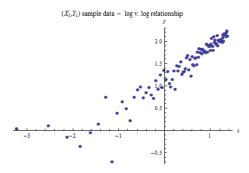


In this case we can attempt to fit the model

$$\log(\hat{Y}) = \hat{\beta}_0 + \hat{\beta}_1 \log(x)$$

watching for the possibility that X_i or the Y_i sample data take negative values.

A final example.



Scatter plot showing log v. log relationship

In this case we can attempt to fit the model

$$e^{\hat{y}} = \hat{\beta}_0 + \hat{\beta}_1 e^x.$$

Although we have solved the least squares problem and found the regression line, we still have many questions to answer.

- usustan erion. To answer these questions requires developing certain statistical tools, the validity of which depend on the following assumptions:

1 the underlying population model is given

$$Y|x = \beta_0 + \beta_1 x + \epsilon$$

- 2 the RV ϵ has $\mathbb{E}[\epsilon] = 0$ and $\operatorname{var}(\epsilon) = \sigma^2$ for all x
- normality normality www. **B** the sample data errors $\epsilon_i \sim \mathsf{N}(\mathbf{0}, \sigma^2)$ and independent so that, $Y_i | X_i \sim \mathsf{N}(\beta_0 + \beta_1 X_i, \sigma^2)$ and independent.

2. Model parameters and estimates

The estimates $\hat{\beta}_0$ and $\hat{\beta}_1$ of the population parameters β_0 and β_1 are themselves RVs – construct a least squares model on a different set of sample data and the estimates will change.

Under the assumptions just stated, these estimates possess some nice statistical properties:

by the Gauss-Markov theorem, these are the minimum variance linear unbiased estimators of the population parameters β₀ and β₁.
 they are the maximum likelihood estimators (MLE).

The first property means that $\mathbb{E}[\hat{\beta}_0] = \beta_0$ and $\mathbb{E}[\hat{\beta}_1] = \beta_1$ (unbiased) and that $\operatorname{var}(\hat{\beta}_0)$ and $\operatorname{var}(\hat{\beta}_1)$ will be smaller than for any other possible estimates $\hat{\beta}_0^*$ and $\hat{\beta}_1^*$.

The second property means, in a "hand waving" sort of way, that they are the estimates that make it most "likely" to observe the sample data (X_i, Y_i) .

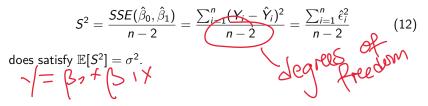
2. Model parameters and estimates

There remains one other population parameter to estimate, the variance σ^2 of the RV ϵ .

One candidate is $\frac{SSE(\hat{\beta}_0,\hat{\beta}_1)}{n}$, with *SSE* given by (3). We used *SSE* to derive our least squares line, and it turns out that this is the MLE of σ^2 .

However it is a **biased** estimate in that $\mathbb{E}[\frac{SSE(\hat{\beta}_0, \hat{\beta}_1)}{n}] \neq \sigma^2$.

It turns out that an **unbiased** version of this estimate can be constructed by taking into account the **degrees of freedom** lost in finding the estimates $\hat{\beta}_0$ and $\hat{\beta}_1$. This estimate



2. Statistical properties of estimates - distributions

It can be shown that $\hat{eta}_0 \sim \mathsf{N}(eta_0,\sigma^2_{\hat{eta}_0})$ with

It inherits its normality from the sample errors ϵ_i , which are assumed to be $N(0, \sigma^2)$. It is unbiased and so has mean β_0 , which we stated before.

 $\sigma_{\hat{\beta}_0}^2 = \sigma^2 \left(\frac{1}{n} + \frac{\overline{X}^2}{S_{XX}}\right). \quad + \quad = \quad$

Similarly, $\hat{\beta}_1 \sim N(\beta_1, \sigma_{\hat{\beta}_1}^2)$ with $\sigma_{\hat{\beta}_1}^2 = \underbrace{\sigma_{\hat{\beta}_1}^2}_{S_{XX}}$

We see that both $\sigma_{\hat{\beta}_0}$ and $\sigma_{\hat{\beta}_1}$ depend on σ – if we don't know the latter we don't know the former.

are both N(0,1), i.e. normally-distributed with zero mean and variance of one.

We can use these RVs as the basis of test statistics in Z-tests and to establish confidence intervals.

However, in practice we will never know the value of $\boldsymbol{\sigma}.$

Instead the sample standard deviation S is used as an approximation of σ .

This gives the unbiased estimates of $\sigma_{\hat{\beta}_0}$

$$S_{\hat{\beta}_0} = \overbrace{S}^{1} \sqrt{\frac{1}{n} + \frac{\overline{X}^2}{S_{XX}}}.$$
 (15)

and of $\sigma_{\hat{\beta}_1}$ $S_{\hat{\beta}_1} = \frac{\textcircled{S}}{\sqrt{S_{XX}}} \tag{16}$

with σ described in (12).

These estimates of $\sigma_{\hat{\beta}_0}$ and $\sigma_{\hat{\beta}_1}$ provide the alternative test statistics

$$T_{\hat{\beta}_0} = \frac{\hat{\beta}_0 - \beta_0}{S_{\hat{\beta}_0}} \tag{17}$$

and

$$T_{\hat{\beta}_1} = \frac{\hat{\beta}_1 - \beta_1}{S_{\hat{\beta}_1}} \tag{18}$$

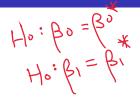
which are both Student's T-distributed with n - 2 degrees of freedom.

These RVs can be used as test statistics in T-tests.

T-test hypotheses

The null hypothesis is

H₀: $eta_j=eta_j^*$, $j\in\{0,1\}$,



with β_i^* some hypothesised level of β_j we hope to exclude.

The alternative hypothesis can be any of

$$H_A$$
: $\beta_j > \beta_j^*$ (upper-tail test)
 H_A : $\beta_j \neq \beta_j^*$ (two-tail test)
 H_A : $\beta_j < \beta_j^*$ (lower-tail test)

R output: *R* reports the results of *T*-tests with $\beta_j^* = 0$.

Test statistic The test statistic $t_{\hat{\beta}_j}^* = \frac{\beta_j - \beta_j^*}{S_{\hat{\alpha}}}$ depends on the sample data, and is a **realisation** of the appropriate RV described in (17)-(18). Rejection of null hypothesis using reject/retain region H_{α} is rejected in favour of H_A at significance level α , $0 < \alpha < 1/2$, if $t^*_{\hat{eta}_j} > t_{1-lpha} \; (ext{upper-tail test})^{\varsigma}$ $|t^*_{\hat{eta}_i}| > t_{1-lpha/2}$ (two-tail test) $t_{\hat{A}_{c}}^{*} < t_{lpha}$ (lower-tail test) where t_{θ} is the **quantile** satisfying $\mathsf{Prob}(T_{\hat{\beta}_i} > t_{\theta}) = \theta.$

x = 0.05 Rejection of null hypothesis using p-value \mathbf{E} quivalently, H_0 is rejected if $p < \alpha$ where the **p-value** $p = \operatorname{Prob}(T_{\hat{\beta}_i} > t^*_{\hat{\beta}_i})$ (upper-tail test) $p = 2 imes \mathsf{Prob}(T_{\hat{eta}_i} > |t^*_{\hat{eta}_i}|)$ (two-tail test) $p = \operatorname{Prob}(T_{\hat{\beta}_i} < t^*_{\hat{\beta}_i})$ (lower-tail test). The null hypothesis H_0 is **retained** in any other case.

Rejection of null hypothesis using Cl Equivalently, H_0 is rejected if β_j^* falls outside the $100(1 - \alpha)$ % Cl for β_j given by $\hat{\beta}_j - S_{\hat{\beta}_j} t_{1-\alpha} \le \beta_j < \infty$ (upper-tail test) $\hat{\beta}_j - S_{\hat{\beta}_j} t_{1-\alpha/2} \le \beta_j \le \hat{\beta}_j + S_{\hat{\beta}_j} t_{1-\alpha/2}$ (two-tail test) $-\infty < \beta_i \le \hat{\beta}_j + S_{\hat{\beta}_i} t_{1-\alpha}$ (lower-tail test).

The null hypothesis H_0 is **retained** in any other case.

Interpretation of special case

When the null hypothesis $\beta_j = 0$ is rejected, we can say the **predictor** x_j is statistically-significant (at significance level α).

2. Statistical properties of model – prediction of $\mathbb{E}[Y|x]$

Recall we set out to model

$$\mathbb{E}[Y|x] = \beta_0 + \beta_1 x$$

$$\approx \hat{\beta}_0 + \hat{\beta}_1 x$$

$$= \hat{Y}|x,$$

with the last being our least squares regression model.

We know this model is unbiased as

$$\mathbb{E}[\hat{Y}|x] = \mathbb{E}[\hat{\beta}_0] + \mathbb{E}[\hat{\beta}_1]x = \beta_0 + \beta_1 x = \mathbb{E}[Y|x]$$

which follows from the unbiased nature of the estimates $\hat{\beta}_0$ and $\hat{\beta}_1$ established earlier.

But $\hat{Y}|x$ is still a RV, so we desire confidence intervals for the values it takes, or the **predictions** it makes of $\mathbb{E}[Y|x]$.

2. Statistical properties of model – prediction of $\mathbb{E}[Y|x]$

Without going into details, we can establish a $100(1 - \alpha)\%$ confidence interval for the model's **prediction** of $\mathbb{E}[Y|x]$ as

$$\hat{Y}|x \pm z_{1-\alpha/2} \times \sqrt{\frac{1}{n} + \frac{(x - \overline{X})^2}{S_{XX}}}$$
(20)

or if σ is unknown as

$$\hat{Y}|x \pm t_{1-\alpha/2} \times S \sqrt{\frac{1}{n} + \frac{(x - \overline{X})^2}{S_{XX}}}$$
(21)

where the quantiles $z_{1-\alpha/2}$ and $t_{1-\alpha/2}$ are associated with the N(0,1) distribution and Students' T distribution with n-2 degrees of freedom respectively.

Again, for the values of α we are interested in, the Student's T-based CI will be wider than the N(0, 1)-based version. This is due to the fatter tails of the Student's-T distribution.

Finally, CIs for the model's **prediction** of Y|x are

$$\hat{Y}|x \pm z_{1-\alpha/2} \times \sigma \sqrt{1 + \frac{1}{n} + \frac{(x - \overline{X})^2}{S_{XX}}}$$
(22)

or if σ is unknown

$$\hat{Y}|x \pm t_{1-\alpha/2} \times S_{V} 1 + \frac{1}{n} + \frac{(x - \overline{X})^2}{S_{XX}}.$$
(23)
Eq. BP = bot B, age
 \hat{P} for a single prison with age 60 (23)
 \hat{P} for a single prison with age 60 (23)
 \hat{P} for the average of a group of ppl (21)
 \hat{P} for the average of a group of ppl (21)
 \hat{P} for the average of a group of ppl (21)

2. Human calculator example

OK, that's a lot of equations. However, we won't be doing the calculations by hand - OK, maybe just one example.

Consider the following data recording the age (X_i) and blood pressure (Y_i) of four individuals.

i	Xi	Y _i
1	39	144
2	47	220
3	45	138
4	47	145

Blood pressure data

We are going to build a model that lets us predict blood pressure from age.

The independent variable in this case is age (X_i) and the dependent variable is blood pressure (Y_i) . (Why?)

Our first step would normally be to plot the data in the hope of spotting a recognisable relationship (linear in the case of simple regression), but with only four data points there isn't much to see.

We suppose that the true relationship between age and blood pressure is

$$Y|x = \beta_0 + \beta_1 x + \epsilon$$

and look to build the model

$$\hat{Y}|x = \hat{\beta}_0 + \hat{\beta}_1 x$$

to approximate

 $\mathbb{E}[Y|x] = \beta_0 + \beta_1 x.$

2. Human calculator example

First we calculate the sample average of the X_i data (average age) $\overline{X} = \frac{39 + 47 + 45 + 47}{4} = 44.5$ and of the Y_i data (average blood pressure) $\overline{Y} = \frac{144 + 220 + 138 + 145}{4} = 161.75.$ Theses sample averages are then used to construct the following table. $X_i \quad Y_i \quad X_i - \overline{X} \quad Y_i - \overline{Y} \quad (X_i - \overline{X})^2 \quad (X_i - \overline{X})(Y_i - \overline{Y})$ 1 39 144 -5.5 -17.7530.25 97.625 2 47 220 2.5 58.25 6.25 145.625 3 45 138 0.5 -23.750.25 -11.8754 47 145 2.5 -16.756.25 -41.875

43.00

189.500

2. Human calculator example

From this table we can read off the figures $S_{XX} = 43$ and $S_{XY} = 189.5$. From (8) we have

$$\hat{\beta}_1 = \frac{S_{XY}}{S_{XX}} = \frac{189.5}{43} \approx 4.41$$

and from (9)

$$\hat{\beta}_0 = \overline{Y} - \hat{\beta}_1 \overline{X} \approx 161.75 - 4.41 \times 44.5 \approx -34.36.$$
 (24)

So our least squares model is

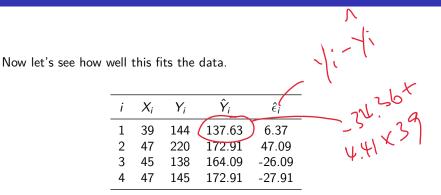
$$\hat{Y}|x = -34.36 + 4.41x$$

or in alternative notation

$$\hat{y}(x) = -34.36 + 4.41x.$$

Obviously, this is not a terribly sophisticated model – for one, it predicts negative blood pressure up until 7.8 years of age.

Be careful extrapolating model outside range of sample data.



Prediction and residual data

Not too well, which is hardly surprising given the amount of data we had.

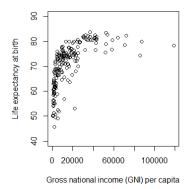
Consider the data set newdata.csv, available in the Week 3 folder on Canvas.

The variables of interest are LifeExp and GNI. We are going to build a model that lets us predict LifeExp from GNI.

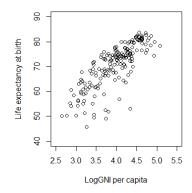
The independent variable in this case is GNI (our X_i values) and the dependent variable is *LifeExp* (our Y_i values).

We would like to build a linear model, so the first thing we do is see if a linear relationship can be found.

We do so with a scatter plot.



We see that no linear relationship is apparent. We perform a log transform of *GNI*, defining the new variable *LogGNI* in the process and create a scatter plot using the new variable.



We now see a reasonable linear relationship and decide to build our model of *LifeExp* against this new variable *LogGNI*.

So we assume an underlying reality of

$$LifeExp|LogGNI = \beta_0 + \beta_1 \times LogGNI + \epsilon$$

and look to build the model

$$\widehat{LifeExp}|LogGNI = \hat{\beta}_0 + \hat{\beta}_1 \times LogGNI$$

as an approximation of

 $\mathbb{E}[LifeExp|LogGNI] = \beta_0 + \beta_1 \times LogGNI.$

To fit a simple linear regression model in R, we use the Im command.

```
> mod1<-lm(newdata$Life_exp ~ newdata$LogGNI)</pre>
```

```
> summary(mod1)
```

```
Coefficients:

Estimate Std. Error t value Pr(>|t|)

(Intercept) 17.2798 2.9577 5.842 2.28e-08 ***

newdata$LogGNI 13.4659 0.7408 18.177 < 2e-16 ***

---

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' '
```

The least squares parameter estimates are $\hat{\beta}_0=17.280$ and $\hat{\beta}_1=13.466,$ resulting in the fitted model

$$\widehat{\text{LifeExp}} = 17.280 + 13.466 \times \text{LogGNI}.$$

As part of its output R reports the p-values associated with T-tests on the parameters β_0 and β_1 .

The hypotheses for the tests on β_0 are

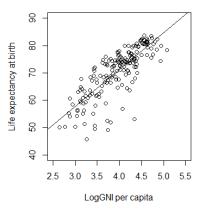
 $\begin{array}{c} H_{0} \colon \ \beta_{0} = 0 \\ H_{A} \colon \ \beta_{0} \neq 0 \end{array}$ and for β_{1} are $\begin{array}{c} H_{0} \colon \ \beta_{1} = 0 \end{array}$

$$H_A: \beta_1 \neq 0.$$

The p-values associated with both of these tests are extremely small so both null hypotheses can be rejected at some significance levels $\alpha < 0.0005.$

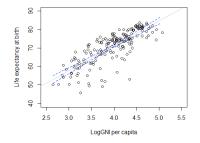
To aid a visual inspection, R will plot the fitted model against sample data using

> abline(mod1)



... and can add 95% confidence bounds for the model's prediction of $\mathbb{E}[\textit{LifeExp}|\textit{LogGNI}]$...

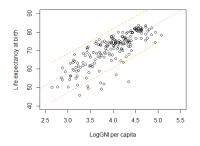
- > newx <- seq(min(newdata\$LogGNI), max(newdata\$LogGNI), by=0.05)</pre>
- > conf_interval <- predict(mod1, newdata=data.frame(LogGNI=newx), interval="confidence", level = 0.95)
- > lines(newx, conf_interval[,2], col="blue", lty=2)
- > lines(newx, conf_interval[,3], col="blue", lty=2)



Regression Line and 95% CI for $\mathbb{E}[LifeExp|LogGNI]$

... and can add 95% confidence bounds for the model's prediction of LifeExp|LogGNI.

```
pred_interval <- predict(mod1, newdata=data.frame(LogGNI=newx),
interval="prediction", level = 0.95)
lines(newx, pred_interval[,2], col="orange", lty=2)
lines(newx, pred_interval[,3], col="orange", lty=2)
```



Regression Line and 95% CI for LifeExp|LogGNI

Of course, there are other questions to answer.

Are the assumptions, on which the statistical tests are built, valid?

How well does the model fit the data?

Is there some non-linear component that can be captured by adding some function of LogGNI as a new variable to the model?

Are there variables other than *LogGNI* that we should consider adding to the model?

We have **interpolated** within the range of the X_i sample data – can we **extrapolate** outside of this range?

We will start to answer some of these questions next week.

- Draper, N. R. and Smith, H. (1998). *Applied regression analysis*. Wiley-Interscience, Somerset, US.
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