## Simple linear regression

# Background.

We all know what a straight line is. Along with the simple way of drawing a line (e.g., by using a ruler), there is a mathematical way to draw a line. This involves specifying the relationship between two **coordinates** *x* (measured on the horizontal or x axis) and *y* (measured on the vertical or y axis). By doing so, each point on the line is "drawn" by specification of the point's coordinates  $(x_i, y_i)$ .

The equation relating the  $x_i$  to the  $y_i$  is as follows:

$$y = \beta_0 + \beta_1 x$$

 $\beta_0$  is called the **intercept** of the line (because if  $x_i=0$  the line "intercepts" the y axis at  $\beta_0$ ), and  $\beta_1$  is called the **slope** of the line.



- **I.** Both lines have the same intercept.
- **II.** Both lines have the same slope (they are **parallel**) but different intercept.
- **III.** Both lines have the same intercept but different **negative** slopes
- **IV.** Both lines have the same (negative) slope but different intercepts.

The appeal of a linear relationship is the *constant slope*. This means that for a fixed increase  $\Delta x$  in x, there will be a fixed change  $\Delta y$  (= $\beta_0 \Delta x$ ). This is going to be a fixed *increase* if the slope is positive, or a fixed *decrease* if the slope is negative, regardless of the value of x. This is in contrast to a *non-linear* relationship, such a *quadratic* or *polynomial*, where for some values of x, y will be increasing, and for some other values y will be decreasing (or vice versa).





Even though it seems upon inspection that y may be increasing for increasing x, the relationship is not a perfect line. If we want to draw a line through the plotted observations that we think best describes the trends in our data we may be confronted with many candidate lines.

## Determining the Best-fitting straight line: The least squares method

Consider the following figure (taken from fitting a regression line to the systolic blood pressure – SBP- data of Table 5-1 in the text):



## The least-squares method

The regression line (whatever it is) will not pass through all data points  $Y_i$ . Thus, in most cases, for each point  $X_i$  the line will produce an *estimated* point  $\hat{Y}_i = \hat{\beta}_0 + \hat{\beta}_1 X_i$  and most probably,  $\hat{Y}_i \neq Y_i$ . In fact, as we see in the previous figure,  $Y_i = \hat{Y}_i + e_i$ . For each choice of  $\hat{\beta}_0$  and  $\hat{\beta}_1$  (note that each pair  $\hat{\beta}_{0}$  and  $\hat{\beta}_{1}$  completely defines the line) we get a new line, and a whole new set of deviation terms  $e_{i}$ . The "best-fitting line" according to the least-squares method is the one that *minimizes* the sum of square deviations  $\sum_{i=1}^{n} \left\| Y_i - \hat{Y}_i \right\|^2 = \sum_{i=1}^{n} e_i^2 = \sum_{i=1}^{n} \left\| Y_i - \left[ \hat{\beta}_0 + \hat{\beta}_1 X_i \right] \right\|^2$ .

## The least-squares method (continued):

The solution is derived by use of calculus. That is, we set the last part of the above equation to zero and take partial derivatives with respect to  $\beta_0$  and  $\beta_1$ .

The resulting *least-squares estimates* of  $\beta_0$  and  $\beta_1$  are given by the following expressions:

$$\hat{\boldsymbol{\beta}}_{1} = \frac{\sum_{i=1}^{n} \left| \boldsymbol{X}_{i} - \overline{\boldsymbol{X}} \right| \left| \boldsymbol{Y}_{i} - \overline{\boldsymbol{Y}} \right|}{\sum_{i=1}^{n} \left| \boldsymbol{X}_{i} - \overline{\boldsymbol{X}} \right|^{2}}, \ \hat{\boldsymbol{\beta}}_{0} = \overline{\boldsymbol{Y}} - \hat{\boldsymbol{\beta}}_{1} \overline{\boldsymbol{X}}$$

Note that since  $\hat{\beta}_0 = \overline{Y} - \hat{\beta}_1 \overline{X}$ , then  $\hat{Y}_i = \hat{\beta}_0 + \hat{\beta}_1 X_i = \overline{Y} + \hat{\beta}_1 \theta X_i - \overline{X}$ . This implies that if  $\hat{\beta}_1$  is close to zero, our best guess for *Y* is the mean  $\overline{Y}$ .

# **Explaining variability**

Statistical modeling is an attempt to "explain" why not all data points are equal. In other words, we are trying to account for the *variability* in the data.

The total variability in the data is given by

$$\sum_{i=1}^{n} \left( Y_{i} - \overline{Y} \right)^{2} = \sum_{i=1}^{n} \left| \left( Y_{i} - \hat{Y}_{i} \right) \right| + \left| \left( \hat{Y}_{i} - \overline{Y} \right) \right|^{2}$$

as we can see by inspection of the previous figure. It also turns out that

$$\sum_{i=1}^{n} \left( Y_{i} - \overline{Y} \right)^{2} = \sum_{i=1}^{n} \left| Y_{i} - \hat{Y}_{i} \right|^{2} + \sum_{i=1}^{n} \left| \hat{Y}_{i} - \overline{Y} \right|^{2}$$

This is because, the cross-product term  $2\sum_{i=1}^{n} \left\| \hat{Y}_{i} - \overline{Y}_{i} \right\| + \hat{Y}_{i} = 0.$ *Proof* (Draper and Smith, p.18): Since,  $\hat{Y}_{i} = \overline{Y} + \hat{\beta}_{1} \theta X_{i} - \overline{X}$  $\hat{Y}_i - \overline{Y} = \hat{\beta}_1 \theta X_i - \overline{X}$  and  $Y_i - \hat{Y}_i = Y_i - \overline{Y} - \hat{\beta}_1 \theta X_i - \overline{X}$ we have,  $2\sum_{i=1}^{n} \left\| \hat{Y}_{i} - \overline{Y} \right\| \left\| Y_{i} - \hat{Y}_{i} \right\| = 2\sum_{i=1}^{n} \hat{\beta}_{1} \ell X_{i} - \overline{X} \right\| \hat{\beta} \ell Y_{i} - \overline{Y} - \hat{\beta}_{1} \ell X_{i} - \overline{X} \right\|$  $= 2\sum_{i=1}^{n} \hat{\beta}_{1} \hat{\beta} \ell X_{i} - \overline{X} \ell Y_{i} - \overline{Y} - \hat{\beta}_{1} \ell X_{i} - \overline{X} \ell Y_{i} - \hat{Y} - \hat{\beta}_{1} \ell X_{i} - \overline{X} \ell Y_{i} - \hat{Y} - \hat{\beta}_{1} \ell X_{i} - \overline{X} \ell Y_{i} - \hat{Y} - \hat{\beta}_{1} \ell X_{i} - \hat{X} \ell Y_{i} - \hat{Y} - \hat{\beta}_{1} \ell X_{i} - \hat{X} \ell Y_{i} - \hat{Y} - \hat{\beta}_{1} \ell X_{i} - \hat{X} \ell Y_{i} - \hat{Y} - \hat{\beta}_{1} \ell X_{i} - \hat{X} \ell Y_{i} - \hat{Y} - \hat{\beta}_{1} \ell X_{i} - \hat{X} \ell Y_{i} - \hat{Y} - \hat{\beta}_{1} \ell X_{i} - \hat{X} \ell Y_{i} - \hat{Y} - \hat{\beta}_{1} \ell X_{i} - \hat{Y} \ell Y_{i} - \hat{Y} - \hat{\beta}_{1} \ell X_{i} - \hat{Y} \ell Y_{i} - \hat{Y} \ell Y_{i} - \hat{\beta}_{1} \ell X_{i} - \hat{Y} \ell Y_{i} - \hat{\beta}_{1} \ell Y_{i$ = 0since  $\hat{\beta}_1 = \frac{\sum\limits_{\substack{\Sigma \\ i=1}}^n |X_i - \overline{X}| |Y_i - \overline{Y}|}{\sum\limits_{\substack{\Sigma \\ \Sigma \\ i=1}}^n |X_i - \overline{X}|^2}$ 

### **Explaining variability (continued)**

This means that there are two parts to the total variability  $SST = \sum_{i=1}^{n} (Y_i - \overline{Y})^2$   $SSY = \sum_{i=1}^{n} (Y_i - \overline{Y})^2$  in the data: one part that is explained or accounted for *due to the regression*  $SSR = \sum_{i=1}^{n} |\hat{Y}_i - \overline{Y}|^2$ , and another that is left unexplained. That is, the regression cannot explain why there are still distances  $SSE = \sum_{i=1}^{n} |Y_i - \hat{Y}_i|^2$  between the estimated points and the data (this is called *error sum of squares*). Since our goal is to reduce the part of the total variability that is unexplained, the regression line will be more useful as the variability due to regression is increasing compared to the unexplained variability. That is, the ratio  $R^2 = \frac{SSR}{SSY} = \frac{SSY - SSE}{SSY}$  is as large as possible.

## **Degrees of freedom**

We define the following quantities

$$1. S_{Y}^{2} = \frac{1}{(n-1)} \sum_{i=1}^{n} (Y_{i} - \overline{Y})^{2} = \frac{1}{(n-1)} SST \quad 2. S_{Y|X}^{2} = \frac{1}{(n-2)} \sum_{i=1}^{n} |Y_{i} - \hat{Y}_{i}|^{2} = \frac{1}{(n-2)} SSE$$

Note that each of the sums of squares that we consider is comprised by a number of terms. For example, the total sum of squares, *SSY* is made up of *n* terms of the form  $(Y_i - \overline{Y})^2$ . Notice however, that once the mean  $\overline{Y}$  has been estimated, only *n*-1 terms are needed to compute *SSY*. The *n*<sup>th</sup> term is known since  $SSY = \sum_{i=1}^{n} ||Y_i - \overline{Y}|| = 0$  for all  $Y_i$ , i=1,...,n-1. The *degrees of freedom* of *SSY* are then *n*-1. On the other hand, the sum of squares due to regression, *SSR*, is computed from a single function involving the  $Y_i$  (the estimated slope  $\hat{\beta}_1$ ), that is,  $SSR = \sum_{i=1}^{n} ||\hat{Y}_i - \overline{Y}||^2 = \hat{\beta}_1^2 \sum_{i=1}^{n} ||X_i - \overline{X}||^2$  and has thus only one degree of freedom associated with it. Finally, *SSE* has *n*-2 degrees of freedom.

Source of	Sums of squares		Mean squares			
variability	(SS)	Df	(MS)	F	Prob > F	
Model	$SSR = \hat{\beta}_1^2 \sum_{i=1}^n \left\  X_i - \overline{X} \right\ ^2$	1	MSR=SSR	$F = \frac{MSR}{MSE}$	$P=\mathbf{P}(F>F_{1, n-2;\alpha})$	
Residual (error)	$SSE = \sum_{i=1}^{n} \left\  Y_i - \hat{Y}_i \right\ ^2$	<i>n</i> -2	$MSE = \frac{SSE}{(n-2)} = S_{Y X}^2$			
Corrected Total	$SSY = \sum_{i=1}^{n} \left\  Y_i - \overline{Y} \right\ ^2$	<i>n</i> -1				



1. The deviations  $\varepsilon_i = Y_i - \hat{Y}$  have zero mean and variance  $s^2$  which is unknown

2. The  $\varepsilon_i$ s are *uncorrelated*, that is, for any *i* and *j* with  $i^{-1}j$ ,  $cov(e_i, e_j)=0$ 

Two immediate implications of these assumptions are that the mean of each data observation is  $E(Y_i) = \mu_{Y|X} = \beta_0 + \beta_1 X_i$ , with *common* variance  $s^2$ , and that  $Y_i$  and  $Y_j$  are uncorrelated for  $i^1 j$ .

A final assumption that allows us to perform statistical tests is as follows:

3. The deviations  $\varepsilon_i$  are distributed according to the normal distribution, with mean 0 and variance  $s^2$  that is,  $\varepsilon_i \sim N(0, s^2)$ .

This final assumption implies that the  $\varepsilon_i$  are not only uncorrelated but also *independent*.

# Inference in simple linear regression

Tests involving the slope of the regression line

Recall that

$$\hat{\beta}_{1} = \sum_{i=1}^{n} \left\| X_{i} - \overline{X} \right\| \left\| Y_{i} - \overline{Y} \right\| / \sum_{i=1}^{n} \left\| X_{i} - \overline{X} \right\|^{2}$$

$$= \sum_{i=1}^{n} \left\| X_{i} - \overline{X} \right\| \left\| Y_{i} / \sum_{i=1}^{n} \left\| X_{i} - \overline{X} \right\|^{2} = \frac{\left\| X_{i} - \overline{X} \right\|}{\sum_{i=1}^{n} \left\| X_{i} - \overline{X} \right\|^{2}} Y_{1} + \dots + \frac{\left\| X_{i} - \overline{X} \right\|}{\sum_{i=1}^{n} \left\| X_{i} - \overline{X} \right\|^{2}} Y_{n}$$
Thus, the variance of  $\hat{\beta}_{1}$  is  $V \left\| \hat{\beta}_{1} \right\| = \frac{\sigma^{2}}{\sum_{i=1}^{n} \left\| X_{i} - \overline{X} \right\|^{2}}$  and the standard deviation is  $S_{\hat{\beta}_{1}} = \frac{\sigma}{\sqrt{\sum_{i=1}^{n} \left\| X_{i} - \overline{X} \right\|^{2}}}$ .  
The solution is left as an exercise. Since  $\sigma^{2}$  is unknown s.e.  $\| \hat{\beta}_{1} \| = \frac{s}{\sqrt{\sum_{i=1}^{n} \left\| X_{i} - \overline{X} \right\|^{2}}}$  is used in the tests

and confidence intervals.

## Test of hypothesis for zero slope

In these models, *y* is our target (or *dependent* variable, the outcome of interest, or a factor that we cannot control but want to explain) and *x* is the explanatory (or *independent* variable).

Within each regression the primary interest is the assessment of the existence of the linear relationship between *x* and *y*. If such an association exists, then *x* provides information about *y*.

Inference on the existence of the linear association is accomplished via tests of hypotheses, and confidence intervals. Both of these center around the estimate of the slope  $\beta$ , since it is clear, that if the slope is zero, then changing *x* will have no impact on *y*, thus there is no association between *x* and *y*.



Confidence intervals of  $\boldsymbol{b}_1$  are constructed as usual, and are based on the standard error of  $\hat{\boldsymbol{\beta}}_1$ , the estimator, and the *t* statistic discussed above.

A  $(1-\alpha)$ % confidence interval is as follows:

$$\hat{\boldsymbol{\beta}}_1 - t_{n-2;(1-\alpha/2)} \mathbf{s.e.} \hat{\boldsymbol{\beta}}_1 , \hat{\boldsymbol{\beta}}_1 + t_{n-2;(1-\alpha/2)} \mathbf{s.e.} \hat{\boldsymbol{\beta}}_1$$

# Inference involving the intercept

In some rare occasions, tests involving the intercept are carried out. Both hypothesis tests and confidence intervals are based on the variance  $S_{\hat{\beta}_{0}}^{2} = \sigma^{2} \left\| \frac{1}{n} + \frac{\overline{X}^{2}}{\Sigma (X_{i} - \overline{X})^{2}} \right\|$ . The derivation is again left as an exercise. (*hint.* Consider the fact that  $\hat{\beta}_{0} = \overline{Y} - \hat{\beta}_{1}\overline{X}$  and that  $\overline{Y}$  and  $\hat{\beta}_{1}$  have zero covariance as it is proven below). The statistic,  $T = \frac{\hat{\beta}_{0}}{s.e.\left|\hat{\beta}_{0}\right|} \sim t_{n-2}$ , where s.e.  $\left|\hat{\beta}_{0}\right| = s \sqrt{\frac{1}{n} + \frac{\overline{X}^{2}}{\Sigma (X_{i} - \overline{X})^{2}}}$ . A (1- $\alpha$ )% confidence interval is as follows:

Inference about the regression line  
Recall that 
$$\hat{Y}_i = \hat{\beta}_o + \hat{\beta}_1 X_i = \overline{Y} + \hat{\beta}_1 (! X_i - \overline{X})!$$
. Thus, the variability of a specific point  $\hat{Y}_o$  at  $X_o$  is given by  
 $S_{\hat{Y}_o}^2 = V(!\overline{Y}] + (!X_o - \overline{X})!^2 V[|\hat{\beta}_1|] + (!X_o - \overline{X}] \operatorname{cov}[|\overline{Y}, \hat{\beta}_1]] = 0.$   
 $= V(!\overline{Y}] + (!X_o - \overline{X})!^2 \sigma^2$   
 $= \sigma^2 \int_{n}^{2} + \frac{(!X_o - \overline{X})!^2 \sigma^2}{\Sigma (!X_i - \overline{X})!^2} = \sigma^2 \int_{n}^{2} \frac{1}{n} + \frac{(!X_o - \overline{X})!^2}{\Sigma (!X_i - \overline{X})!^2} \int_{n}^{2} \frac{1}{n} + \frac{(!X_o - \overline{X})!^2}{\Sigma (!X_i - \overline{X})!^2} \int_{n}^{2} \frac{1}{n} + \frac{(!X_o - \overline{X})!^2}{\Sigma (!X_i - \overline{X})!^2} \int_{n}^{2} \frac{1}{n} + \frac{(!X_o - \overline{X})!^2}{\Sigma (!X_i - \overline{X})!^2} \int_{n}^{2} \frac{1}{n} + \frac{(!X_o - \overline{X})!^2}{\Sigma (!X_i - \overline{X})!^2} \sigma^2 = 0$ 



This interval is wider away from the mean of the X's, and narrower closer to that mean.



### An *F* test of overall linear association (continued)

The *F* test of linear association, that is, the test of whether a line (other than the horizontal one going through the sample mean of the *Y*'s) is useful in explaining some of the variability of the data is based on the observation that the expected value  $E[|MSR|] = \sigma^2 + \beta_1^2 \sum ||X_i - \overline{X}||^2$  while  $E[|SSE|] = E[|S_{Y|X}|] = \sigma^2$  when the regression model is correctly specified (we will see what happens when this is not the case). If the population regression slope  $\beta_1 \approx 0$ , that is, if the regression does not add anything new to our understanding of the data (does not explain a substantial part of the variability), the two mean square errors *MSR* and *MSE* are estimating a common quantity (the population variance  $\sigma^2$ ).

Thus the ratio should be close to 1 if the hypothesis of no linear association between *X* and *Y* is present. On the other hand, if a linear relationship exists, ( $\beta_1$  is far from zero) then *SSR*>*SSE* and the ratio will deviate significantly from 1.



The *F* test of hypothesis of no linear association is defined as follows:

1. 
$$H_0$$
: No linear association exists between X and Y

2.  $H_a$ : A linear association exists between X and Y

3. Tests are carried out at the  $(1-\alpha)$ % level of significance

4. The test statistic is  $F = \frac{MSR}{MSE}$ .

5. **Rejection rule:** Reject H<sub>o</sub>, if  $F > F_{1, n-2;\alpha}$ . This will happen if *F* is far from 1.0.

In simple linear regression, the F test is equivalent to the t test for zero slope described earlier. In

fact,  $T^2 = F$  where  $T^2$  is distributed according to a  $t_{n-2}$  and F according to an  $F_{1,n-2}$ .

Analysis of the systolic blood pressure example								
In this exa	mple, the relation	onship betwee	n systolie	c blood pressure	(SBP) and age is explore	ed. The		
data are lis	ted below.							
. list								
	sbp	age		sbp	age			
1.	144	39	16.	130	4			
2.	220	47	17.	135	45			
3.	138	45	18.	114	17			
4.	145	47	19.	116	20			
5.	162	65	20.	124	19			
б.	142	46	21.	136	36			
7.	170	67	22.	142	50			
8.	124	42	23.	120	39			
9.	158	67	24.	120	21			
10.	154	56	25.	160	44			
11.	162	64	26.	158	53			
12.	150	56	27.	144	63			
13.	140	59	28.	130	29			
14.	110	34	29.	125	25			
15.	128	42	30.	175	69			



. reg sbp a	age						
Source	SS	df	MS		Number of obs	=	30
+-					F(1, 28)	= 21	.33
Model	6394.02269	1 6	394.02269		Prob > F	= 0.00	001
Residual	8393.44398	28 2	99.765856		R-squared	= 0.43	324
+-					Adj R-squared	= 0.41	121
Total	14787.4667	29 5	09.912644		Root MSE	= 17.3	314
======================================	Coef.	Std. Er	 r. t	 P> t	[95% Conf.	Interva	 al]
age	.9708704	.210215	7 4.618	0.000	.5402629	1.4014	 478
_cons	98.71472	10.0004	7 9.871	0.000	78.22969	119.19	997

### Conclusions

1. MSR=6394.02269

- 2. *MSE*=299.765856, which is the best estimate of  $\sigma^2$  if the model is correct.
- 3. F=21.33 which is much larger than the tail of  $F_{1,28;0.95}$ . We thus reject the null hypothesis of no linear association between blood pressure and age.
- 4. The t statistic of zero slope is T=4.618. This is much larger than a t<sub>28;0.975</sub>. Alternatively, the p value of the test is 0.000<0.05=α. Thus, we again *reject* the hypothesis of no linear association between systolic blood pressure and age. In fact, the positive estimate of the regression slope β<sub>1</sub> = 0.9709 means that blood pressure *increases* with age (about one unit for every year of life).
  5. The R<sup>2</sup> =0.4324. This means that approximately 43% of the variability (in the subjects' blood pressure) was explained by the regression model (i.e., age). Note the entry for *adjusted* R<sup>2</sup>. This

is a quantity such that adj.  $R^2 = \frac{SSE/(n-2)}{SSY/(n-1)} = 1 - \left[1 - R^2\right] \left[\frac{(n-1)}{(n-2)}\right] = 0.4121$ . The adjusted  $R^2$  is

supposed to be used to compare between several models of varying complexity. It is not used often.



The option c(l.) means that the sbphat points should be connected by a line, while the sbp points should be left unconnected (a scatter plot) respectively while the option s(io) means that no symbol should be used for sbphat points while a small circle should be used for sbp points.

## Confidence intervals about the regression line

Since STATA does not automatically produce 95% confidence intervals about the regression line these must be generated manually. To do this, we must first calculate the standard error of each estimated value, s.e.  $\left\|\hat{Y}_{o}\right\| = s \sqrt{\frac{1}{n} + \frac{\left|\hat{X}_{o} - \overline{X}\right|^{2}}{\sum \left|X_{i} - \overline{X}\right|^{2}}}$ . This is computed by the option stdp after the

predict command

```
. predict s, stdp
```

Then, the 95% upper and lower limits in each case are produced as follows:

- . gen ul=sbphat+invt(28,0.95)\*s
- . gen ll=sbphat-invt(28,0.95)\*s

In each case, invt(28,0.95) is the *two-sided* 95% tail of a  $t_{28}$  distribution (i.e., the inverse *t*).



## **Additional topic: Prediction**

Statistical modeling does not only attempt to explain variability in the data, but *predict* a future observation  $\hat{Y}_{X_o}$  at  $X_o$ . In doing so, it is critical to consider the sources of possible variability that enter into this prediction.



## **Prediction intervals**

When talking about future observations, we cannot construct "confidence intervals" in the strict sense (since the new observation is not a population parameter). The similar concept is called a "prediction interval". A  $(1-\alpha)$ % such interval is based on the estimated standard deviation

s.e. 
$$\|\hat{Y}_{X_o}\| = s \sqrt{1 + \frac{1}{n} + \frac{\|X_o - \overline{X}\|^2}{\sum \|X_o - \overline{X}\|^2}}$$
 and is constructed as follows:  
$$\|\hat{Y}_{X_o} - t_{n-2;(1-\alpha/2)} \text{s.e.}\|\hat{Y}_{X_o}\|, \hat{Y}_{X_o} + t_{n-2;(1-\alpha/2)} \text{s.e.}\|\hat{Y}_{X_o}\|\|$$



```
. gen llpred=sbphat-invt(28,0.95)*sr
```

In each case, invt(28,0.95) is the *two-sided* 95% tail of a  $t_{28}$  distribution (i.e., the inverse *t*).

