Correlation and Regression

- a *scatterplot* is used to assess the relationship between two variables
- each point shows the values of the two variables (x_i, y_i) measured on the same individual
- look for the overall pattern and for striking deviations from it
- two variables are associated if some values of one variable tend to occur more often with some values of the the other variable
- can describe the *form*, *direction* and *strength* of any association
 - form can be *linear* or *nonlinear*, positive or negative

- sometimes we hope to explain one variable by the other
 - we call them the *response* and *explanatory* variables
 - the response variable is shown on the vertical axis
- we may want to explain or predict the useable volume in board feet/10 of a tree given a measurement at chest height in inches

```
MTB > set c1
DATA> 36 28 28 41 19 32 22 38 25 17 31 20 25 19 39 33 17 37 23 39
DATA> set c2
DATA> 192 113 88 294 28 123 51 252 56 16 141 32 86 21 231 187 22 205 57 265
MTB > name c1 'diameter'
MTB > name c2 'volume'
MTB > plot c2 c1
      300+
 volume
      200+
      100 +
                    2
               2
        0 +
                                                                  ----diameter
                             25.0
        15.0
                   20.0
                                        30.0
                                                  35.0
                                                             40.0
```

Correlation

- the correlation coefficient measures the direction and strength of the linear association between two quantitative variables
- given data $(x_i, y_i), i = 1 \dots n$, the correlation coefficient is

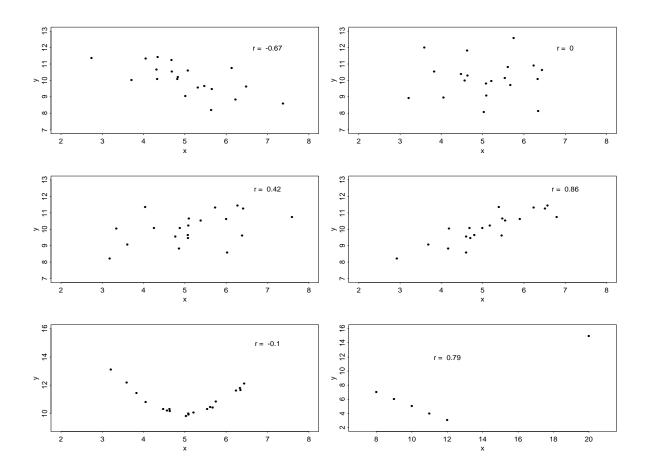
$$r = \frac{1}{n-1} \sum \left(\frac{x_i - \bar{x}}{s_x}\right) \left(\frac{y_i - \bar{y}}{s_y}\right)$$

- the product of the two terms in braces is positive if both x_i and y_i are above or below their means
- r must be between -1 and 1
- r = 0 means no linear association
- r = 1(-1) means all points fall on a line with positive (negative) slope
- calculating correlation coefficient in MINITAB

MTB > corr c1 c2

Correlation of diameter and volume = 0.976

some sample plots



- top left moderately strong negative linear association (r = -.67)
- top right no association (r = 0)
- middle left weak positive association (r = .42)
- middle right strong positive association (r = .86)

- bottom left strong quadratic association (zero linear, r = 0)
- bottom right perfect negative association with one influential outlier (r = .79)

Alternative Formulae

• the numerator of the formula for r is

$$SS_{XY} = \sum_{i=1}^{n} (x_i - \bar{x})(y_i - \bar{y})$$

• SO

$$r = \frac{1}{n-1} \frac{SS_{XY}}{s_x s_y}$$

• we can also write

$$SS_{XX} = \sum_{i=1}^{n} (x_i - \bar{x})^2$$

and

$$s_x = \sqrt{\frac{SS_{XX}}{n-1}}$$

SO

$$r = \frac{SS_{XY}}{\sqrt{SS_{XX}SS_{YY}}}$$

where SS_{YY} is defined similarly to SS_{XX}

• note that SS_{XY} can be written in various ways

$$SS_{XY} = \sum_{i=1}^{n} (x_i - \bar{x}) y_i$$

= $\sum_{i=1}^{n} x_i (y_i - \bar{y})$
= $\sum_{i=1}^{n} x_i y_i - n \bar{x} \bar{y}$
= $\sum_{i=1}^{n} x_i y_i - \sum_{i=1}^{n} x_i \sum_{i=1}^{n} y_i / n$

the version to use depends on what you are given

Example: To study the effect of ozone pollution on soybean yield, data were collected at four ozone dose levels and the resulting soybean seed yield monitored. Ozone dose levels (in ppm)were reported as the average ozone concentration during the growing season. Soybean yield was reported in grams per plant.

X	Υ
Ozone(ppm)	Yield (gm/plant)
.02	242
.07	237
.11	231
.15	201

 to calculate the correlation coefficient by hand, we obtain the squares and cross products and their sums

Х	Y	X^2	Y^2	XY
.02	242	.0004	58564	4.84
.07	237	.0049	56169	16.59
.11	231	.0121	53361	25.41
.15	201	.0225	40401	30.15

• Column sums: $\sum x_i = .35$, $\sum y_i = 911$, $\sum x_i^2 = .0399$, $\sum y_i^2 = 208, 495$, and $\sum x_i y_i = 76.99$

- \bullet Means: $\bar{x}=.0875$ and $\bar{y}=227.95$
- Intermediate terms:

$$SS_{xx} = \sum_{i} (x_i - \bar{x})^2 = \sum_{i} x_i^2 - \frac{(\sum x_i)^2}{n}$$
$$= .0399 - \frac{(.35)^2}{4} = .009275$$

$$SS_{yy} = \sum_{i} (y_i - \bar{y})^2 = \sum_{i} y_i^2 - \frac{(\sum y_i)^2}{n}$$
$$= 208,495 - \frac{(911)^2}{4} = 1014.75$$

and

$$SS_{xy} = \sum_{i} (x_i - \bar{x})(y_i - \bar{y})$$

= $\sum_{i} x_i y_i - \frac{(\sum x_i)(\sum y_i)}{n}$
= $76.99 - \frac{.35(911)}{4} = -2.7225$

• the correlation coefficient is

$$r = \frac{SS_{XY}}{\sqrt{SS_{XX}SS_{YY}}} = \frac{-2.7225}{\sqrt{.009275(1014.75)}} = -.8874$$

• there is a strong negative linear association between yield and ozone

Simple Linear Regression

- a line summarizing the relationship between two variables
- has form $y = \beta_0 + \beta_1 x$
 - must choose which variable is the response y and which the explanatory variable x
 - β_0 is the y-intercept, the value for y when x = 0
 - β_1 is the slope, the change in y for a unit change in x
- can be used to predict value of \boldsymbol{y} for a given \boldsymbol{x}
- obtain by minimizing the sum of squares of vertical deviations from the line

$$SSE = \sum_{i=1}^{n} (y_i - \beta_0 - \beta_1 x_i)^2$$

• note that SSE is a function of β_0 and β_1 only because the data (x_i, y_i) , $i = 1, \ldots, n$ is known • the least squares slope has a surprisingly simple formula

$$\hat{\beta}_1 = r \frac{s_y}{s_x}$$

• the fitted intercept is

$$\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x}$$

• the equation of the least squares line is

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

$$= \bar{y} - \hat{\beta}_1 \bar{x} + \hat{\beta}_1 x$$

$$= \bar{y} + \hat{\beta}_1 (x - \bar{x})$$

$$= \bar{y} + r \frac{s_y}{s_x} (x - \bar{x})$$

- from the latter formula, we see that the fitted value when $x = \bar{x}$ is \bar{y} , so the least squares line always goes through the point \bar{x}, \bar{y}
- rearranging further, we get

$$\frac{y - \bar{y}}{s_y} = r \frac{x - \bar{x}}{s_x}$$

• this gives another interpretation of the correlation coefficient, namely that it is the slope of the best fitting line if both the x and y variables are standardized

Example: for the tree data, $\bar{y} = 123.0$, $\bar{x} = 28.45$, r = .976, $s_y = 91.7$ and $s_x = 8.11$

• the estimated slope is

$$\hat{\beta}_1 = rs_y/s_x = .976(91.7)/8.11 = 11.036$$

• the estimated intercept is

$$\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x} = 123.0 - 11.036(28.45)$$

= -190.96

the fitted line is

volume = -190.96 + 11.036 diameter

- if the diameter were 27 inches, we would predict a volume of 107.012 board feet/10)
- these results differ from MINITAB due to round-off error

MTB > regress c2 1 c1; SUBC> residuals c3. The regression equation is volume = - 191 + 11.0 diameter

Predictor	Coef	Stdev	t-ratio	р
Constant	-191.12	16.98	-11.25	0.000
diameter	11.0413	0.5752	19.19	0.000

s = 20.33 R-sq = 95.3% R-sq(adj) = 95.1%

Analysis of Variance

SOURCE	DF	SS	MS	F	р
Regression	1	152259	152259	368.43	0.000
Error	18	7439	413		
Total	19	159698			

Example: For the ozone data,

•
$$\hat{\beta}_1 = \frac{SS_{xy}}{SS_{xx}} = -293.531$$

• $\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x} = 227.95 - (-293.531)(.0875) = 253.434$

• the least squares line is

$$y\hat{ield} = 253.434 - 293.531ozone$$

Derivation of formulae for intercept and slope

- those who have taken calculus will know that one can use derivatives to find the maximum or minimum of a function
- in this case there are two variables β_0 and β_1 , and so both *partial* derivatives can be set to zero and solved
- the partial derivatives are

$$\frac{\partial SSE}{\partial \beta_0} = -2\sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_i)$$

and

$$\frac{\partial SSE}{\partial \beta_1} = -2\sum_{i=1}^n x_i(y_i - \beta_0 - \beta_1 x_i)$$

 when equated to zero and rearranged, these give the so-called "normal equations".

$$n\beta_0 + \beta_1 \sum_{i=1}^n x_i = \sum_{i=1}^n y_i$$

and

$$\beta_0 \sum_{i=1}^n x_i + \beta_1 \sum_{i=1}^n x_i^2 = \sum_{i=1}^n x_i y_i$$

- (the term 'normal' here has nothing to do with the normal distribution, but rather to the geometric idea of orthogonality or perpendicularity)
- the two normal equations are solved simultaneously to obtain

$$\hat{\beta}_1 = \frac{SS_{XY}}{SS_{XX}}$$

and

$$\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x}$$

- there is a second derivation which doesn't require calculus
- notice that SSE is a quadratic function of β_0 and β_1
- first consider β_1 to be fixed and find the value of β_0 which minimizes SSE

completing the square and summing gives

$$SSE = A\beta_0^2 + B\beta_0 + C$$

where

$$A = n$$

$$B = 2\beta_1 \sum x_i - 2\sum y_i$$

$$C = \sum y_i^2 - 2\beta_1 \sum x_i y_i + \beta_1^2 \sum x_i^2$$

• the minimum of a quadratic occurs at -B/2A, so whatever the value of β_1 the best choice for β_0 is

$$\beta_0 = \frac{-2\beta_1 \sum x_i + 2\sum y_i}{2n}$$
$$= \bar{y} - \beta_1 \bar{x}$$

• now substitute this choice into SSE, so that it is now a quadratic function of β_1 only

$$SSE = \sum_{i=1}^{n} (y_i - (\bar{y} - \beta_1 \bar{x}) - \beta_1 x_i)^2$$

$$= \sum_{i=1}^{n} (y_i - \bar{y} - \beta_1 (x_i - \bar{x}))^2$$
$$= A\beta_1^2 + B\beta_1 + C$$

• where now

$$A = SS_{XX}$$
$$B = -2SS_{XY}$$
$$C = SS_{YY}$$

• the minimum occurs at

$$\hat{\beta}_1 = \frac{-B}{2A} = \frac{SS_{XY}}{SS_{XX}}$$

• substituting in β_0 gives

$$\hat{\beta}_1 = \bar{y} - \hat{\beta}_1 \bar{x}$$