Multiple Linear Regression Example

N = 28 standsy = vol/ha (m3)

volume/ha	Age	Site	Basal area/ha	Stems	Top height	Qdbh
m ³	years	Index	m ²	/ha	m	cm
559.3	82	14.6	32.8	1071	22.4	22.2
559	107	9.4	44.2	3528	17	9.3
831.9	104	12.8	50.5	1764	21.5	17
365.7	62	12.5	29.6	1728	16.4	12.1
454.3	52	14.6	35.4	2712	18.9	14.1
486	58	13.9	39.1	3144	17.5	14
441.6	34	18.5	36.2	3552	17.4	13.8
375.8	35	17	33.4	4368	15.6	12.2
451.4	33	19.1	35.4	2808	16.8	14.7
419.8	23	23.4	34.4	3444	17.3	14
467	33	17.7	42	6096	16.4	12.2
288.1	33	15	30.3	5712	13.8	5.6
306	32	18.2	27.4	3816	16.7	12.5
437.1	68	13.8	33.3	2160	19.1	16.2
633.2	126	11.4	39.9	1026	21	23.2
707.2	125	13.2	40.1	552	23.3	29.2
203	117	13.7	11	252	22.1	25.8
915.6	112	13.9	48.7	1017	24.2	25
903.5	110	13.9	51.5	1416	23.2	23
883.4	106	14.7	49.4	1341	24.3	23.7
586.5	124	12.8	35.2	2680	22.6	21.5
500.1	60	18.4	27.3	528	22.7	24.4
343.5	63	14	26.9	1935	17.6	14.1
478.6	60	15.2	34	2160	19.4	9.9
652.2	62	15.9	42.5	1843	20.5	13.2
644.7	63	16.2	40.4	1431	21	16.1
390.8	57	14.8	30.4	2616	18.3	13.9
709.8	87	14.3	42.3	1116	22.6	23.9

Multiple Linear Regression Example

Objective: obtain an equation for estimating volume per ha from some of the easy to measure variables such as

- -stems/ha
- basal area /ha (only need dbh on each tree)
- qdbh (need dbh on each tree and stems/ha)

VERY IMPORTANT assumption of MLR: The relationship between the x's and y is linear!

Transformations

- Same as for SLR except that there are more x variables; can also add variables e.g. use dbh and dbh² as x1 and x2.
- Try to transform x's first and leave y = variable of interest; not always possible.
- Use graphs to help choose transformations

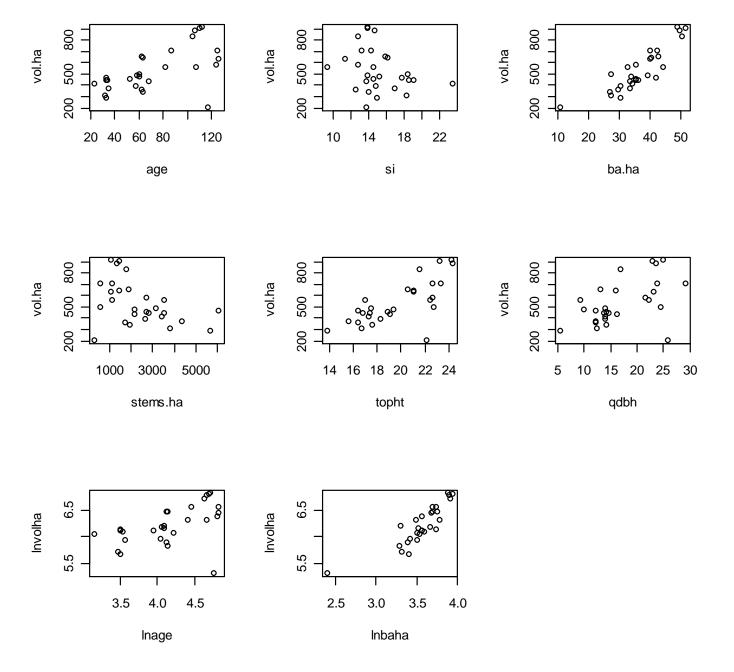
R code

```
> standdat<- read.table("../data/stand.txt",header=TRUE)</pre>
> # since standdat was created as a dataframe, the names can be attached for simpler commands
> attach(standdat) # this allows you to use the dataframe, treedat, with shorter names for
   variables
> names(standdat)
[1] "vol.ha" "age"
                        "si"
                                     "ba.ha" "stems.ha" "topht"
                                                                      "qdbh"
>
> lnvolha=log(vol.ha)
> lnage=log(age)
> lnbaha=log(ba.ha)
>
> detach(standdat) # This just detaches the dataframe, standdat, but it can be reattached
> standdat<-data.frame(standdat,lnvolha,lnage,lnbaha)
> rm(lnvolha,lnage,lnbaha)
>
> attach(standdat)
> names(standdat)
 [1] "vol.ha" "age"
                                      "ba.ha"
                                                "stems.ha" "topht"
     "qdbh" "lnvolha" "lnage"
                                      "lnbaha"
>
```

Script 4_MLR.R

plots

```
> par(mfrow=c(3,3),cex=0.7)
> plot(vol.ha~age,data=standdat)
> plot(vol.ha~si,data=standdat)
> plot(vol.ha~ba.ha,data=standdat)
> plot(vol.ha~stems.ha,data=standdat)
> plot(vol.ha~topht,data=standdat)
> plot(vol.ha~qdbh,data=standdat)
> plot(lnvolha~lnage,data=standdat)
> plot(lnvolha~lnage,data=standdat)
> par(mfrow=c(1,1),cex=1)
>
```



Multiple Linear Regression (MLR)

Population:
$$y_i = \beta_0 + \beta_1 x_{1i} + \beta_2 x_{2i} + ... + \beta_p x_{mi} + \varepsilon_i$$

Sample:
$$y_i = b_0 + b_1 x_{1i} + b_2 x_{2i} + ... + b_p x_{mi} + e_i$$

$$\hat{y}_i = b_0 + b_1 x_{1i} + b_2 x_{2i} + \dots + b_m x_{mi}$$
 $e_i = y_i - \hat{y}_i$

- θ_0 is the y intercept parameter
- $\theta_1, \theta_2, ..., \theta_p$ are slope parameters
- $x_{1i}, x_{2i}, ..., x_{mi}$ are independent variables
- ε_i is the error term or the residual; is the variation in the dependent variable (the y) which is not accounted for by the independent variables (the x's).

Multiple Linear Regression (MLR)

For any fitted equation (we have the estimated parameters), we can get the *estimated* average for the dependent variable, for any set of x's. This will be the "predicted" value for y, which is the estimated average of y, given the particular values for the x variables.

Finding the Set of Coefficients that Minimizes the Sum of Squared Errors

- Same process as for SLR: Find the set of coefficients that results in the minimum SSE, just that there are more parameters, therefore more partial derivative equations and more equations
- E.g., with 3 x-variables, there will be 4 coefficients (intercept plus 3 slopes) so four equations
- For linear models, there will be one unique mathematical solution.

Least squares solution for MLR

Find the set of estimated parameters (coefficients) that minimize sum of squared errors

$$\min(SSE) = \min(\sum_{i=1}^{n} e_i^2)$$

$$= \min\left(\sum_{i=1}^{n} \left(y_i - (b_0 + b_1 x_{1i} + b_2 x_{2i} + \dots + b_p x_{mi})\right)^2\right)$$

Take **partial derivatives** with respect to each of the coefficients, set them equal to zero and solve.

For three x-variables we obtain:

$$b_0 = \overline{y} - b_1 \overline{x}_1 - b_2 \overline{x}_2 - b_3 \overline{x}_3$$

$$b_{1} = \frac{SPx_{1}y}{SSx_{1}} - b_{2} \frac{SPx_{1}x_{2}}{SSx_{1}} - b_{3} \frac{SPx_{1}x_{3}}{SSx_{1}}$$

$$b_2 = \frac{SPx_2y}{SSx_2} - b_1 \frac{SPx_1x_2}{SSx_2} - b_3 \frac{SPx_2x_3}{SSx_2}$$

$$b_{3} = \frac{SPx_{3}y}{SSx_{3}} - b_{1}\frac{SPx_{1}x_{3}}{SSx_{3}} - b_{2}\frac{SPx_{2}x_{3}}{SSx_{3}}$$

SP = sum of products between two variables, for example for *y* with x1:

$$SPx_1 y = \sum_{i=1}^n (y_i - \overline{y})(x_{1i} - \overline{x}_1)$$

$$= \sum_{i=1}^n y_i x_{1i} - \frac{\left(\sum_{i=1}^n x_{1i}\right)\left(\sum_{i=1}^n y_i\right)}{n} = s^2_{x_1 y}(n-1)$$

SS = sum of squares for one variable, for example for x1:

$$SSx_1 = \sum_{i=1}^n (x_{1i} - \overline{x}_1)^2 = \sum_{i=1}^n x_{1i}^2 - \frac{\left(\sum_{i=1}^n x_{1i}\right)^2}{n} = s^2_{x_1}(n-1)$$

Then, we would need: SSY, SSX₁, SSX₂, SSX₃, SPX₁Y, SPX₂Y, SPX₃Y, SPX₁X₂, SPX₁X₃, SPX₂X₃, and insert these into the four equations and solve:

$$b_0 = \bar{y} - b_1 \bar{x}_1 - b_2 \bar{x}_2 - b_3 \bar{x}_3$$

$$b_{1} = \frac{SPx_{1}y}{SSx_{1}} - b_{2} \frac{SPx_{1}x_{2}}{SSx_{1}} - b_{3} \frac{SPx_{1}x_{3}}{SSx_{1}}$$

$$b_2 = \frac{SPx_2y}{SSx_2} - b_1 \frac{SPx_1x_2}{SSx_2} - b_3 \frac{SPx_2x_3}{SSx_2}$$

$$b_3 = \frac{SPx_3y}{SSx_3} - b_1 \frac{SPx_1x_3}{SSx_3} - b_2 \frac{SPx_2x_3}{SSx_3}$$

And then check assumptions, make any necessary transformations, and start over!

Properties of a least squares regression "surface":

- 1. Always passes through $(\overline{x}_1, \overline{x}_2, \overline{x}_3, ..., \overline{x}_m, \overline{y})$
- 2. Sum of residuals is zero, i.e., $\Sigma e_i = 0$
- 3. SSE the least possible (least squares)
- 4. The slope for a particular x-variable is AFFECTED by correlation with other x-variables: CANNOT interpret the slope for a particular x-variable, UNLESS it has zero correlation with all other x variables (or nearly zero if correlation is estimated from a sample).

Meeting assumptions of MLR

Once coefficients are obtained, we must **check the assumptions of MLR** before we can:

- assess goodness of fit (i.e., how well the regression line fits the sample data)
- test significance of the regression
- calculate confidence intervals and test hypotheses

For these tests to be valid, assumptions of MLR concerning the observations and the errors (residuals) must be met.

Residual Plots

Assumptions of:

- 1. The relationship between the x's and y is linear VERY IMPORTANT!
- The variances of the y values must be the same for every combination of the x values.
- 3. Each observation (i.e., x_i 's and y_i) must be independent of all other observations.

can be visually checked by using **RESIDUAL PLOTS**

A residual plot shows the residual (i.e., $y_i - \hat{y}_i$) as the y-axis and the predicted value (\hat{y}_i) as the x-axis.

THIS IS THE SAME as for SLR. Look for problems as with SLR. The effects of failing to meet a particular assumption are the same as for SLR

What is different? Since there are many x variables, it will be harder to decide what to do to fix any problems.

Normality Histogram or Plot

A fourth assumption of the MLR is:

4. The y values must be normally distributed for each combination of x values.

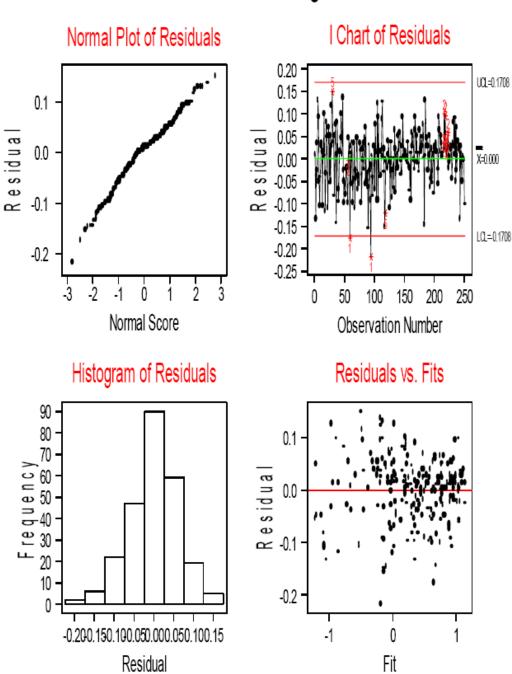
A histogram of the errors and/or a normality plot can be used to check this, as well as tests of normality as with SLR. Failure to meet these assumptions will result in the same problems as with SLR

Residual Model Diagnostics

Example:

- Linear relationship met
- equal variance met
- no evidence of trend with observation number (independence maybe met).
- normal distribution met

Logvol=f(dbh,logdbh)



Volume versus dbh

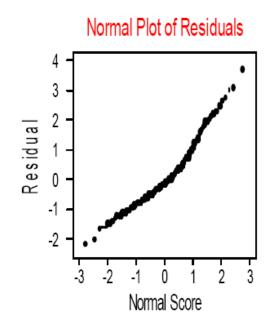
Example:

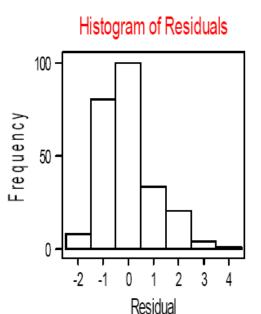
 Independence of observations not met

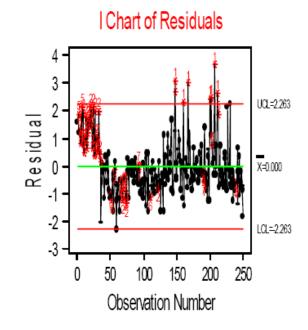
When we have no time relation in sequence of sampling (order in space or time), there is no reason to suspect relationship among our observations

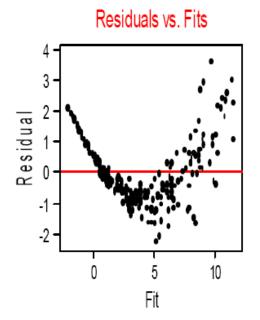
Linear relationship not met:

Pos. and neg. residuals are not balanced for all values of ŷ







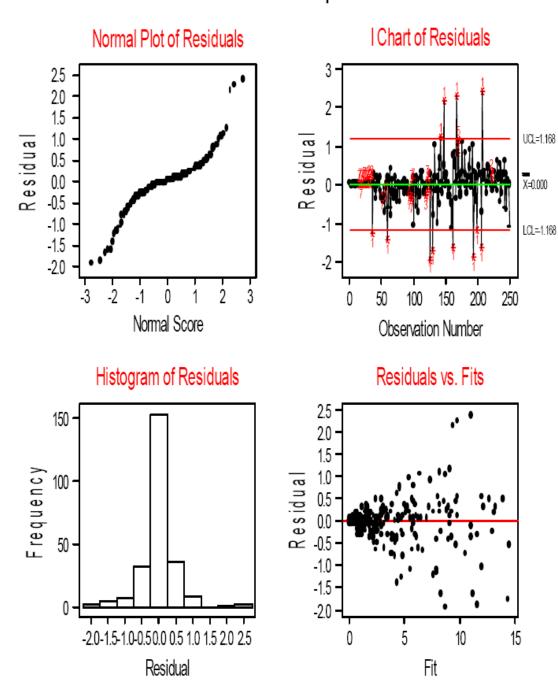


Volume versus dbh squared and dbh

Example:

Variances are not equal:

The spread of the residuals is not the same for all ŷ



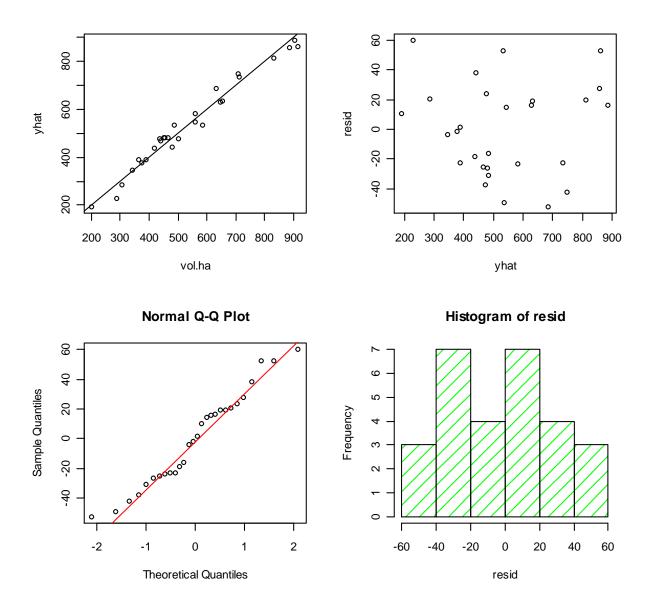
```
> yhat<-fitted(model.volha)</pre>
> resid<-resid(model.volha)</pre>
> par(mfrow=c(2,2),cex=0.7)
> plot(yhat~vol.ha)
> abline(a=0,b=1) # plot a reference line where yhat equals vol.ha
> plot(resid~yhat) # residual plot
>
> qqnorm(resid) # normality plot
> qqline(resid, col=2)
> hist(resid, breaks =6 , density=10,col="green", border="black") # draws a histogram
> par(mfrow=c(1,1),cex=1)
> shapiro.test(resid)
        Shapiro-Wilk normality test
data: resid
W = 0.9606, p-value = 0.36
```

Normal distribution of the residuals:

H0: Residuals are Normally distributed (this is what we hope)

Ha: Residuals are not Normal

If P-value $< \alpha$, then we reject the H0



Measurements and Sampling Assumptions

The remaining assumptions of MLR are based on the measurements and collection of the sampling data, as with SLR

- 5. The x values are measured without error (i.e., the x values are fixed).
- 6. The y values are randomly selected for each given set of the x variables (i.e., for each fixed set of x values, a list of all possible y values is made).

As with SLR, often observations will be gathered using simple random sampling or systematic sampling (grid across the land area). This does not strictly meet this assumption [much more difficult to meet with many x variables!] If the equation is "correct", then this does not cause problems. If not, the estimated equation will be biased.

"iterative" process:

- 1. Fit the equation
- 2. Check the assumptions [and check for outliers]
- Make any transformations based on the residual plot, and plots of y versus each x
- 4. Also, check any very unusual points to see if these are measurement/transcription errors; ONLY remove the observation if there is a very good reason to do so
- 5. Fit the equation again, and check the assumptions
- 6. Continue until the assumptions are met [or nearly met]

Careful with transformations!

Example:

Predicted $log10(vol) = -4.2 + 2.1 \times log10(dbh) + 1.1 \times log10(height)$

where $b_0 = -4.2$; $b_1 = 2.1$; $b_2 = 1.1$ estimated by finding the least squared error solution.

Using this equation for dbh =30 cm, height=28m, logten(dbh) =1.48, logten(height) =1.45; logten(vol) = 0.503. ∴ volume (m³) = 3.184. This represents the estimated average volume for trees with dbh=30 cm and height=28 m.

Note: This equation is originally a nonlinear equation:

$$vol = a \times dbh^b \times ht^c \times \varepsilon$$

Which was transformed to a linear equation using logarithms:

 $log10(vol) = log10(a) + b log10(dbh) + c log10(ht) + log10\varepsilon$

And this was fitted using multiple linear regression

For the observations in the sample data used to fit the regression, we can also get an estimate of the error (we have measured volume).

If the measured volume for this tree was 3.000 m³, or **0.477** in log10 units:

$$error = y_i - \hat{y}_i = 0.477 - 0.503 = -0.026$$

For the fitted equation using log10 units.

In original units, the estimated error is 3.000-3.184= - 0.184

NOTE: This is not simply the antilog of -0.026.

Measures of Goodness of Fit

How well does the regression fit the sample data?

- For multiple linear regression, a graph of the predicted versus measured y values indicates how well the line fits the data
- Two measures commonly used: coefficient of multiple determination (R²) and standard error of the estimate(SE_F), similar to SLR.

To calculate R² and SE_E

First calculate SSE, SSy and SSreg:

SSE (this is what was minimized):

$$SSE = \sum_{i=1}^{n} e_i^2 = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$
$$= \sum_{i=1}^{n} (y_i - (b_0 + b_1 x_{1i} + b_2 x_{2i} + \dots b_m x_{mi}))^2$$

The sum of squared differences between the measured and estimated y's. This is the same as for SLR, but there are more slopes and more x (predictor) variables

To calculate R² and SE_E

SSy: the sum of squares for y:

$$SSy = \sum_{i=1}^{n} (y_i - \overline{y})^2 = s_y^2 (n-1)$$

The sum of squared difference between the measured y and the mean of y-measures.

NOTE: In some texts, this is called the **sum of squares total (SSTO)**.

To calculate R² and SE_E

• *SSreg*: the sum of squares regression:

$$SSreg = \sum_{i=1}^{n} (\bar{y} - \hat{y}_i)^2 = b_1 SPx_1 y + b_2 SPx_2 y + \dots + b_3 SPx_3 y$$
$$= SSy - SSE$$

The sum of squared differences between the mean of y-measures and the predicted y's from the fitted equation.

= the sum of squares for y – the sum of squared errors.

Remarkable property

$$(Y_i - \bar{Y})^2 = (\hat{Y}_i - \bar{Y})^2 + (Y_i - \hat{Y}_i)^2$$

Or SSy = SSreg + SSe

Breakdown of Degrees of Freedom

- SSY (=SSTO)
 - 1 linear constraint due to the calculation and inclusion of the mean (equivalently: because sum must be 0)
 - n-1 degrees of freedom
- SSE
 - m + 1 linear constraints arising from the estimation of m + 1 parameters in the regression function
 - n-(m +1) = n-m-1 degrees of freedom
- SSR
 - All fitted values are calculated from the same regression function: m + 1 degrees of freedom in the regression parameters, one is lost due to linear constraint $\sum_{(\hat{n})=\bar{n}}^{n}$
 - m degrees of freedom

Remarkable:
$$n - 1 = (n - m - 1) + m$$

R^2

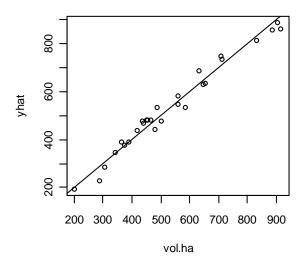
$$R^{2} = \frac{SSy - SSE}{SSy} = 1 - \frac{SSE}{SSy} = \frac{SSreg}{SSy}$$

- SSE, SSY are based on y's used in the equation will not be in original units if y was transformed
- R^2 = coefficient of multiple determination; proportion of variance of y, accounted for by the regression using x's
- 0 (when SSy = SSE) (very poor horizontal surface representing no relationship between y and x's) to 1 (perfect fit – surface passes through the data)

$$R^2$$

$$R^{2} = \frac{SSy - SSE}{SSy} = 1 - \frac{SSE}{SSy} = \frac{SSreg}{SSy}$$

 It can be shown that the coefficient of multiple determination R² can be viewed as a coefficient of simple determination r² between the responses y_i and the fitted values ŷ_i



Adjusted R² value

SSE falls as *m* (*number of independent variables*) increases, so R² rises as more explanatory (independent or predictor) variables are added.

Adjusted R² value adjusts by dividing each sum of squares by its associated degrees of freedom

 \rightarrow A penalty is added as you add x-variables to the equation:

$$R_{a}^{2} = 1 - \frac{SSE}{\frac{N - (m+1)}{SSy}} = 1 - \left(\frac{n-1}{n - (m+1)}\right) \frac{SSE}{SSy}$$

SE_E = Standard Error of the Estimate

$$SE_E = \sqrt{\frac{SSE}{n-m-1}}$$

- = root of the mean square error (MSE)
- SSE is based on y's used in the equation will not be in original units if y was transformed
- n m 1 is the degrees of freedom of the error; is the number of observations minus the number of fitted coefficients
- SE_F standard error of the estimate; in same units as y

SE_F = Standard Error of the Estimate

$$SE_E = \sqrt{\frac{SSE}{n-m-1}}$$

- Under normality of the errors:
 - $-\pm 1$ SE_F $\cong 68\%$ of sample observations
 - $-\pm 2$ SE_F $\cong 95\%$ of sample observations
- Want low SE_F

y-variable was transformed

- Can calculate estimates of r² and SE_E for the original y-variable unit, in order to compare to R² and SE_E of other equations where the y was not transformed, similar to SLR
- Estimated r²: I² (Fit Index)

$$I^2 = 1 - SSE/SSY$$

- where SSE, SSY are in original units. NOTE must "backtransform" the predicted y's to calculate the SSE in original units.
- Does not have the same properties as R², however: it can be less than 0

y-variable was transformed

Estimated standard error of the estimate (SE_F'):

$$SE_E' = \sqrt{\frac{SSE(original\ units)}{n-m-1}}$$

- SE_E' standard error of the estimate; in same units as original units for the dependent variable
- want low SE_E'

```
> summary(model.volha)
Call:
lm(formula = vol.ha ~ ba.ha + stems.ha + qdbh)
Residuals:
                                                Multiple
   Min 10 Median 30 Max
                                                coefficient of
-52.334 -23.875 -0.104 19.642 59.953
                                                determination
Coefficients:
             Estimate Std. Error t value **Ir(>|t|)
(Intercept) -1.982e+02 4.789e+01 -4.138 0.000372 ***
        1.857e+01 7.564e-01 24/546 < 2e-16 ***
ba.ha
stems.ha -3.124e-02 7.016e-03 -4.453 0.000167 ***
qdbh 7.542e+00 1.740e+00 4.335 0.000225 ***
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 '' 1
                                                                   = SE<sub>F</sub>
                                                                   = root MSE
Residual standard error, 33.43 on 24 degrees of freedom
Multiple R-squared: 0.9727, Adjusted R-squared: 0.9692
F-statistic: 284.6 on 3 and 24 DF, p-value: < 2.2e-16
```

Testing whether the Regression is Significant

- Does knowledge of x's improve the estimate of the mean of y?
- Or is it a flat surface, which means we should just use the mean of y as an estimate of y for any x?

Mean Square (MS)

- = Sum of Squares divided by it's associated degrees of freedom
- MSE = SSE/ (n m 1):

Called the **Mean squared error**, as would be the average of the squared error if we divided by *n*.

Instead, we divide by n-m-1. Why? The degrees of freedom are n-(m+1); n observations with m+1 statistics estimated from these, b_0 , b_1 , b_2 , ... b_m

Under the assumptions of MLR, is an unbiased estimated of the true variance of the error terms (error variance)

• MSR = SSR/m:

Called the Mean Square Regression

Degrees of Freedom=m: m x-variables

Under the assumptions of MLR, this is an estimate of the error variance PLUS a term of variance explained by the regression using x.

Expected Mean Squares

(statistical theory provides these results:)

$$E\{MSE\} = \sigma^{2}$$

$$E\{MSR\} = \sigma^{2} + SSreg$$

- mean of sample distribution of MSE = σ^2 Independent of linear relationship X's~Y Independent of $\beta_1 = \beta_2 = \beta_3 = ... = \beta_m = 0$ or not all slopes =0
- mean of sample distribution of MSR = σ^2 if $\beta_1 = \beta_2$ = $\beta_3 = ... = \beta_m = 0$

Regression significant?

HO: Regression is not significant

H1: Regression is significant

Same as:

H0: $\beta_1 = \beta_2 = \beta_3 = ... = \beta_m = 0$ [all slopes are zero meaning no relationship with x's]

H1: not all slopes = 0 [some or all slopes are not equal to zero] If H0 is true, then the equation is:

$$y_i = \beta_0 + \theta x_{1i} + \theta x_{2i} + \dots + \theta x_{mi} + \varepsilon_i$$
$$y_i = \beta_0 + \varepsilon_i \qquad \hat{y}_i = \beta_0$$

Where the x-variables have no influence over y; they do not help to better estimate y

Analysis of Variance approach

As with SLR, we can use an F-test, as it is the ratio of two variances; unlike SLR we cannot use a t-test since we are testing several slope coefficients

Using an F test statistic:
$$F = \frac{SSreg/m}{SSE/(n-m-1)} = \frac{MSreg}{MSE}$$

If F is 1 \rightarrow no relationship

• Under H0, this follows an F distribution for a 1- α percentile with m and n-m-1 degrees of freedom

if F is bigger than 1 \rightarrow there is a relationship

 If the F for the fitted equation is larger than the F from the table, we reject H0 (not likely true). The regression is significant, in that one or more of the true slopes (the population slopes) are likely not equal to zero

Information for the F-test in the Analysis of Variance Table:

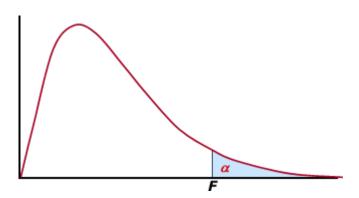
Source	df	SS	MS	F	p-value
Regression	m	SSreg	MSreg= SSreg/m	F= MSreg/MSE	Prob F> $F_{(\mathbf{m},n-m-1,1-\alpha)}$
Error	<i>n-m-</i> 1	SSE	MSE = SSE/(m-1)	n	
Total	n-1	SSy			

Is the regression significant?

H0: $\beta_1 = \beta_2 = \beta_3 = ... = \beta_m = 0$ regression is not significant

H1: not all slopes = 0 regression is significant

→ F-test



Two ways to look:

- 1) If F-value > critical F-value, then reject H0 F-value ? \rightarrow summary(model.volha) \rightarrow F-statistic: 284.6 F_c = F_{m,n-m-1,1-\alpha} \quad \alpha=0.05 \rightarrow using the table (or R function) m=3; n=28; n-m-1=24 \quad > qf (0.95,3,24) \quad [1] 3.008787
- 2) OR if P-value < α , then reject H0 P-value? \rightarrow summary(model.volha) \rightarrow p-value: < 2.2e-16

```
> summary(model.volha)
Call:
lm(formula = vol.ha ~ ba.ha + stems.ha + qdbh)
Residuals:
   Min
           10 Median 30
                                 Max
-52.334 -23.875 -0.104 19.642 59.953
Coefficients:
             Estimate Std. Error t value Pr(>|t|)
(Intercept) -1.982e+02 4.789e+01 -4.138 0.000372 ***
ba.ha
         1.857e+01 7.564e-01 24.546 < 2e-16 ***
stems.ha -3.124e-02 7.016e-03 -4.453 0.000167 ***
qdbh
         7.542e+00 1.740e+00 4.335 0.000225 ***
Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 '' 1
Residual standard error: 33.43 on 24 degrees of freedom
Multiple R-squared: 0.9727, Adjusted R-squared: 0.9692
F-statistic: 284.6 on 3 and 24 DF p-value: < 2.2e-16
                  DF of SSR
                               DF of SSE
> qf(0.95,3,24)
```

[1] 3.008787

```
> anova(model.volha)
Analysis of Variance Table
                              partial SSRegressions
Response: vol.ha
          Df Sum Sq Mean Sq F value
                                         Pr(>F)
             756843 4756843 677.122 < 2.2e-16 ***
ba.ha
                                                           MLR ANOVA table: R
stems.ha
           1 176537
                     176537 157.942 4.774e-12 ***
                                                            decomposes SSR in parts
                       21009 18.796 0.0002251 ***
qdbh
              21009
                                                            that sum up to SSR!
Residuals 24
              26826
                       1118
                 0 \*** 0 SSE for the full model (24 df)
Signif. codes:
> anovatable <- anova(model.volha)</pre>
> ssr <- sum(anovatable[1:3,2])</pre>
> ssr
[11 954388.9
> dfr <- sum(anovatable[1:3,1])</pre>
> dfr
[1] 3
> msr <- ssr/dfr
> msr
[1] 318129.6
> mse <- anovatable[4,3]</pre>
> mse
[1] 1117.735
> fvalue <- msr/mse</pre>
                                    Same result as in summary()
> fvalue
[1] 284.6199
```

Estimated Standard Errors for the Slope and Intercept

Under the assumptions, we can obtain an unbiased estimate of the standard errors for the slope and for the intercept [measure of how these would vary among different sample sets], using the one set of sample data.

For multiple linear regression, these are more easily calculated using matrix algebra. If there are more than 2 x-variables, the calculations become difficult; we will rely on statistical packages to do these calculations.

Confidence Intervals for the True Slope and Intercept

Under the assumptions, confidence intervals can be calculated as:

For
$$\beta_0$$
: $b_0 \pm t_{1-\alpha/2, n-m-1} \times s_{b_0}$

For
$$\beta_j$$
: $b_j \pm t_{1-\alpha/2, n-m-1} \times s_{b_j}$ [for any of the slopes]

Hypothesis Tests for one of the True Slopes or Intercept

- H0: βj = c [the parameter (true intercept or true slope is equal to the constant, c, given that the other x-variables are in the equation]
- H1: βj ≠ c [true intercept or slope differs from the constant c; given that the other x-variables are in the equation]

Hypothesis Tests for one of the True Slopes or Intercept

Test statistic:

$$t = \frac{b_j - c}{s_{b_i}}$$

Under H0, this is distributed as a t value of $t_c = t_{n-m-1, 1-\alpha/2}$. Reject H0 if $|t| > t_c$.

 It is possible to do one-sided hypotheses also, where the alternative is that the true parameter (slope or intercept) is greater than (or less than) a specified constant c. MUST be careful with the t_c as this is different.

The regression is significant, but which x-variables should we retain?

With MLR, we are particularly interested in which x variables to retain. We then test: Is variable x_j significant given the other x variables? e.g. diameter, height - do we need both?

H0: $\beta_j = 0$, given other x-variables (i.e., variable not significant)

H1: $\beta_j \neq 0$, given other x-variables.

A t-test for that variable can be used to test this.

→ T-test

```
> summary(model.volha)
                                                           H0: \beta_0 = 0
Call:
                                                           \text{Ha}: \beta_0 \neq 0
lm(formula = vol.ha ~ ba.ha + stems.ha + qdbh)
                                                           t - statistic: \frac{-(198.2e + 02) - 0}{47.89e + 01}
Residuals:
    Min 10 Median 30
                                    Max
-52.334 -23.875 -0.104 19.642 59.953
                                                           if |t| > t_{critical}, we reject H0
Coefficients:
                                                           this is the same as Pv < \alpha
              Estimate Std. Error t value Pr(>|t|)
(Intercept) -1.982e+02 4.789e+01 -4.138 0.000372 ***
                                                           We don't really care about
ba.ha 1.857e+01 7.564e-01 24.546 < 2e-16 ***
                                                           the intercept: no x-variable is
stems.ha -3.124e-02 7.016e-03 -4.453 0.000167 ***
                                                           associated with it
qdbh 7.542e+00 1.740e+00 4.335 0.000225 ***
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 '' 1
Residual standard error: 33.43 on 24 degrees of freedom
Multiple R-squared: 0.9727, Adjusted R-squared: 0.9692
F-statistic: 284.6 on 3 and 24 DF, p-value: < 2.2e-16
```

Partial F-test

Partial F-test can be used to test one x-variable (as t-test) or to test a group of x-variables, given the other x-variables in the equation

- Get regression analysis results for all x-variables [full model]
- Get regression analysis results for all but the xvariables to be tested [reduced model]

H0: the dropped variables are not significant, the slopes are all zero

H1: not all the slopes of the dropped variables are zero

Partial F-test

$$partial F = \frac{\left(SSreg(full) - SSreg(reduced)\right)/r}{SSE/(n-m-1)(full)}$$

OR

$$partial F = \frac{\left(SSE(reduced) - SSE(full)\right)/r}{SSE/(n-m-1)(full)}$$

$$= \frac{\left(SS \text{ due to dropped variable(s)}\right)/r}{MSE(full)}$$

Where *r* is the number of x-variables that were dropped also equals:

- (1) the regression degrees of freedom for the full model minus the regression degrees of freedom for the reduced model,
- OR (2) the error degrees of freedom for the reduced model, minus the error degrees of freedom for the full model

Partial F-test

- Under H0, this follows an F distribution for a 1-α percentile with r and n-m-1 (full model) degrees of freedom
- If the partial F is larger than the critical F-value from the table, we reject H0 (not likely true).
 The contribution of the dropped variables is significant, in that one or more of the true slopes are likely not equal to zero

→ partial F-test:

In R we can perform partial F-tests by fitting both the reduced and full models separately and thereafter comparing them using anova (reduced, full).

→ partial F-test:

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→ partial F-test:

In R we can perform partial F-tests by fitting both the reduced and full models separately and thereafter comparing them using anova (reduced, full).

```
> model.volha<-lm(vol.ha~ba.ha+stems.ha+qdbh)</pre>
> model.volha2<-lm(vol.ha~ba.ha+stems.ha)</pre>
> anova(model.volha2, model.volha)
                                                    # partial F test to compare the two
    nested models
Analysis of Variance Table
Model 1: vol.ha ~ ba.ha + stems.ha
Model 2: vol.ha ~ ba.ha + stems.ha + qdbh
  Res.Df RSS of Sum of Sq
                                Sum of Squares Error (Residuals):
      25 47835
                       21009 1: -Reduced model
      24 26826
                                -Full model
Signif. codes:
                 0 '***' 0.001
                                \rightarrow MSE (full) = 26826/24 = 1117.75
```

→ partial F-test:

In R we can perform partial F-tests by fitting both the reduced and full models separately and thereafter comparing them using anova (reduced, full).

```
> model.volha<-lm(vol.ha~ba.ha+stems.ha+qdbh)</pre>
> model.volha2<-lm(vol.ha~ba.ha+stems.ha)</pre>
> anova(model.volha2, model.volha)
                                                   # partial F test to compare the two
   nested models
                                     Partial SSregression for the omitted term:
Analysis of Variance Table
                                     (SSR(full)-SSR(reduced)
Model 1: vol.ha ~ ba.ha + stems.ha
Model 2: vol.ha ~ ba.ha + stems.ha
                                      qdbh
  Res.Df RSS Df Sum of Sq
                                        Pr(>F)
      25 47835
                             18.796 0.0002251 ***
      24 26826
                       21009
Signif. codes:
                         0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

The output shows t

Degrees of freedom of Partial SSregression = number of omitted terms: 1

(p-

value=0.0002251) we can reject the null hypothesis (p3 = 0) at the 5% level of significance. It appears that the variable qdbh contributes significant information to the vol/ha once the variables ba.ha and stems/ha have been taken into consideration.

→ partial F-test:

In R we can perform partial F-tests by fitting both the reduced and full models separately and thereafter comparing them using anova (reduced, full).

```
> model.volha<-lm(vol.ha~ba.ha+stems.ha+qdbh)</pre>
> model.volha2<-lm(vol.ha~ba.ha+stems.ha)</pre>
> anova(model.volha2, model.volha)
                                                  # partial F test to compare the two
   nested models
Analysis of Variance Table
                                               F = [(SSR(full)-SSR(reduced))/r]/MSE(full)
                                               F = [21009/1]/[26826/24]
Model 1: vol.ha ~ ba.ha + stems.ha
                                               F = 18.796
Model 2: vol.ha ~ ba.ha + stems.ha + qdbh
  Res.Df RSS Df Sum of Sq
                                       Pr (>F)
      25 47835
1
      24 26826 1
                      21009 18.796 0.0002251 ***
Signif. codes:
                0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

→ partial F-test:

In R, Partial F-values for single x-variables are given in the anova table of the full model!

```
> anova(model.volha)
Analysis of Variance Table
                              partial SSRegressions
Response: vol.ha
          Df Sum Sq Mean Sq F value
                                         Pr(>F)
             756843 4756843 677.122 < 2.2e-16 ***
ba.ha
                                                           MLR ANOVA table: R
stems.ha
           1 176537
                     176537 157.942 4.774e-12 ***
                                                            decomposes SSR in parts
                       21009 18.796 0.0002251 ***
qdbh
              21009
                                                            that sum up to SSR!
Residuals 24
              26826
                       1118
                 0 \*** 0 SSE for the full model (24 df)
Signif. codes:
> anovatable <- anova(model.volha)</pre>
> ssr <- sum(anovatable[1:3,2])</pre>
> ssr
[11 954388.9
> dfr <- sum(anovatable[1:3,1])</pre>
> dfr
[1] 3
> msr <- ssr/dfr
> msr
[1] 318129.6
> mse <- anovatable[4,3]</pre>
> mse
[1] 1117.735
> fvalue <- msr/mse</pre>
                                    Same result as in summary()
> fvalue
[1] 284.6199
```

→ partial F-test:

Sometimes we are interested in simultaneously testing whether a certain subset of the coefficients are equal to 0 (e.g. β 3 = β 4 = 0).

```
> model.volha3<-lm(vol.ha~ba.ha+stems.ha+qdbh+age+si)</pre>
> anova(model.volha, model.volha3)
                                                 # partial F test to compare the two
   nested models
Analysis of Variance Table
Model 1: vol.ha ~ ba.ha + stems.ha + qdbh
                                                          \beta3 = \beta4 = 0, if the other
Model 2: vol.ha ~ ba.ha + stems.ha + qdbh + age + si
  Res.Df
        RSS Df Sum of Sq F Pr(>F)
                                                          variables are included in the
      24 26826
                                                          model
      22 23200 2 3625.6 1.719 0.2025
> model.volha4<-lm(vol.ha~ba.ha+stems.ha+qdbh+aqe+topht)
> anova(model.volha, model.volha4)
                                                 # partial F test to compare the two
   nested models
Analysis of Variance Table
Model 1: vol.ha ~ ba.ha + stems.ha + qdbh
Model 2: vol.ha ~ ba.ha + stems.ha + qdbh + age + topht
                                                          Not all of β3 and β4 are 0, if the
          RSS Df Sum of Sq F
  Res.Df
                                      Pr(>F)
                                                          other variables are included in the
      24 26826
      22 11744 2 15082 14.127 0.0001132 ***
                                                          model
Signif. codes:
                0 \***' 0.001 \**' 0.01 \*' 0.05 \.' 0.1 \' 1
```

Confidence Interval for the True Mean of y given a particular set of x values

For the mean of all possible y-values given a particular value set of x-values ($\mu_v | \mathbf{x_h}$):

$$\hat{y} \mid \mathbf{x}_h \pm t_{n-m-1,1-\alpha/2} \times s_{\hat{y} \mid \mathbf{x}_h}$$

Where
$$\hat{y} \mid \mathbf{x}_h = b_0 + b_1 x_{1h} + b_2 x_{2h} + \dots + b_m x_{mh}$$

$$s_{\hat{y}|\mathbf{x}_h}$$
 = from statistical package output

Confidence Bands: Plot of the confidence intervals for the mean of y for several sets x-values is not possible with MLR

Confidence Interval for 1 or more y-values given a particular set of x values

For one possible new y-value given a particular value set of x-values :

$$\hat{y}_{(new)} \mid \mathbf{x}_h \pm t_{n-m-1,1-\alpha/2} \times s_{\hat{y}(new)\mid \mathbf{x}_h}$$

Where

$$\hat{y} \mid \mathbf{x}_h = b_0 + b_1 x_{1h} + b_2 x_{2h} + \dots + b_m x_{mh}$$

 $s_{\hat{y}(new)|\mathbf{x}_h}$ = from statistical package output

Confidence Interval for 1 or more y-values given a particular set of x values

For the average of g new possible y-values given a particular value of x :

$$\hat{y}_{(new)} \mid \mathbf{x}_h \pm t_{n-m-1,1-\alpha/2} \times s_{\hat{y}(newg)\mid \mathbf{x}_h}$$

Where

$$\hat{y} \mid \mathbf{x}_h = b_0 + b_1 x_{1h} + b_2 x_{2h} + \dots + b_m x_{mh}$$

 $s_{\hat{y}(newg)|\mathbf{x}_h}$ = from statistical package output

Given stems/ha=300, qdbh=20 cm, and ba/ha=20 m2/ha, what is the estimated volume per ha? How would you get a CI for this estimate?

The function **predict()** can be used to make

- confidence intervals for the mean response : option interval="confidence".
- prediction intervals: option interval="prediction"

By default this makes 95% confidence and prediction intervals.

If you instead want to make a 99% confidence or prediction interval use the option level=0.99.

```
> model.volha<-lm(vol.ha~ba.ha+stems.ha+qdbh)
> predict(model.volha,data.frame(stems.ha=300, ba.ha=20,
        qdbh=20),interval="confidence")
        fit lwr upr
1 314.6161 279.4611 349.7711
> predict(model.volha,data.frame(stems.ha=300, ba.ha=20,
        qdbh=20),interval="prediction")
        fit lwr upr
1 314.6161 237.1754 392.0569
```

A 95% confidence interval of the mean is given by (279, 349)

A 95% prediction interval is given by (237,392). Note that this is quite a bit wider than the confidence interval, indicating the variation about the mean.

Selecting and Comparing Alternative Models

Process to Fit an Equation using Least Squares Steps (same as for SLR):

- Sample data are needed, on which the dependent variable and all explanatory (independent) variables are measured.
- 2. Make any transformations that are needed to meet the most critical assumption: The relationship between y and x's is linear. Example: volume = $\beta_0 + \beta_1$ dbh + β_2 dbh² may be linear whereas volume versus dbh is not. Need both variables.
- 3. Fit the equation to minimize the sum of squared error.
- 4. Check Assumptions. If not met, go back to Step 2; try a number of equations.
- 5. If assumptions are met, then check if the regression is significant. If it is not, then it is not a candidate model (need other x-variables). If yes, then go through further steps for MLR.

- 6. Are all variables needed? If there are x-variables that are not significant, given the other variables:
- drop the <u>least significant</u> one (highest p-value, lowest F, or lowest absolute value of t)
- refit the regression and check assumptions.
- if assumptions are met, then repeat steps 5 and 6

continue until all variables in the regression are significant given the other x-variables also in the model

Variable selection

In many situations the set of predictor variables to be included is not predetermined

→ selecting predictor variables becomes part of the analysis.

Two main approaches towards variable selection:

- all possible regressions approach
 considers all possible subsets of the pool of explanatory variables and finds the
 model that best fits the data according to some criteria (e.g. Adjusted R2, AIC and
 BIC). These criteria assign scores to each model and allow us to choose the model
 with the best score.
- 2. automatic methods (algorithm) useful when the number of explanatory variables is large and it is not feasible to fit all possible models.

Methods have been developed to help in choosing which x-variables to include in the equation. These include:

1. R² (or Adjusted R²). The equation is fitted for a number of combinations of the x-variables to predict y. The ones with the highest R² are reported. CAUTION: You must check the assumptions of these fitted equations by fitting the equation with variables given. If assumptions are NOT met, these are NOT candidate models EVEN with a high R². ALSO, consider costs of measuring the x-variables, significance of the x-variables (given the other variables) etc. This only gives some ideas of models to try.

2. Stepwise.

- 1) The most important variable is added to the model (highest partial F-value or absolute value of t; has lowest p-value).
- 2) Each of the other variables are added; the next most important variable is added to the model
- 3) Repeat Step 2
- 4) At any time, a variable already entered in, may become not significant. Drop it, and continue with Step 2.
- 5) Continue until all variables in the regression are significant, and the ones that are not in the equation are not significant, given the ones that are in the equation.

NOTES:

 This just gives candidate models. You must check whether the assumptions are met and do a full assessment of the regression results

3. Backwards Stepwise:

- 1) All x-variables are added to the model
- 2) Check to see if variables are not significant given the other variables in the equation (use partial F-test or t-test)
- 3) If all x-variables are significant given the other variables, stop.
 Otherwise, drop the variable with the lowest partial F-value (highest p-value)
- 4) Repeat step 2, until all variables in the equation are significant, given the other variables that are in the equation

NOTES:

- This again just gives candidate models. You must check whether the assumptions are met and do a full assessment of the regression results
- Unlike "stepwise", once a variable is dropped, it cannot come back in, even
 if it might be significant with a different set of x-variables than when it was
 dropped.

4. Forward Stepwise: This is the same as Stepwise, EXCEPT, that once a x-variable is added to the model, it is not removed, even if it becomes non-significant at a particular step in the process.

NOTES:

 This again just gives candidate models. You must check whether the assumptions are met and do a full assessment of the regression results

Steps for Forward Stepwise, for example:

To fit this "by hand", you would need to do the following steps:

- 1. Fit a simple linear regression for vol/ha with each of the explanatory (x) variables.
- 2. Of the equations that are significant (assumptions met?), select the one with the highest F-value.
- 3. Fit a MLR with vol/ha using the selected variable, plus each of the explanatory variables (2 x-variables in each equations). Check to see if the "new" variable is significant given the original variable (which may now be not significant, but forward stepwise does not drop variables). Of the ones that are significant (given the original variable is also in the equation), pick the one with the largest partial-F (for the new variable).
- 4. Repeat step 3, bringing in variables until i) there are no more variables or ii) the remaining variables are not significant given the other variables.

R-code Stepwise

```
> null <- lm(vol.ha ~ 1,data = standdat)</pre>
> summary(null)
                  Script 5 MLR variableselection.R
Call:
lm(formula = vol.ha ~ 1, data = standdat)
Residuals:
   Min 1Q Median 3Q Max
-332.54 -122.99 -53.24 111.04 380.06
Coefficients:
           Estimate Std. Error t value Pr(>|t|)
(Intercept) 535.54 36.03 14.87 1.6e-14 ***
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1
1 / 1
Residual standard error: 190.6 on 27 degrees of freedom
```

R-code Stepwise

```
> null <- lm(vol.ha ~ 1,data = standdat)</pre>
> summary(null)
                     Script 5 MLR variableselection.R
> mean(vol.ha)
              > sem <- sd(vol.ha)/sqrt(length(vol.ha))</p>
 [1] 535.5393
               > sem
               [1] 36.02642
Residuals:
              10 Median
    Min
                               3Q
                                     > t.value <- (mean(vol.ha)-0)/sem
                           111.04
-332.54 -122.99
                 -53.24
                                     > t.value
                                     [1] 14.86518
Coefficients:
             Estimate Std. Error t value Pr(>|t|)
                        36.03
                                    14.87 1.6e-14 ***
(Intercept)
               535.54
                    > sd(vol.ha-mean(vol.ha))
                           > 2*pt(t.value,df=length(vol.ha)-1,lower.tail=FALSE)
 [1] 190.6339
                           [1] 1.601009e-14
Residual standard error: 190.6 on 27 degrees of freedom
```

```
> full <- lm(vol.ha ~ .,data = standdat)</pre>
> summary(full)
Call:
lm(formula = vol.ha ~ ., data = standdat)
Residuals:
   Min 1Q Median 3Q Max
-32.269 - 15.239 - 1.759 14.183 51.850
Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept) -5.523e+02 7.991e+01 -6.912 7.9e-07 ***
age 3.135e-01 4.665e-01 0.672 0.508860
si 2.778e+00 3.814e+00 0.728 0.474492
ba.ha 1.648e+01 6.747e-01 24.423 < 2e-16 ***
stems.ha -1.443e-02 6.326e-03 -2.281 0.033114 *
topht 2.316e+01 4.991e+00 4.640 0.000141 ***
qdbh 2.808e-03 2.041e+00 0.001 0.998915
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 '
1 1
Residual standard error: 23.35 on 21 degrees of freedom
Multiple R-squared: 0.9883, Adjusted R-squared: 0.985
F-statistic: 296.3 on 6 and 21 DF, p-value: < 2.2e-16
```

R-code Stepwise

```
null <- Im(vol.ha ~ 1,data = standdat)
summary(null)
full <- Im(vol.ha ~ .,data = standdat)
summary(full)

step.model1 <- step(null, scope=list(lower=null, upper=full), direction="forward")
summary(step.model1)
step.model2 <- step(full,direction=c("backward"))
summary(step.model2)
step.model3 <- step(null, scope = list(upper=full), direction=c("both"))
summary(step.model3)</pre>
```

AIC represents a trade-off between the goodness of fit of the model and the complexity of the model.

AIC can tell nothing about the quality of the model in an absolute sense. If all the candidate models fit poorly, AIC will not give any warning of that.

```
> library(leaps) #Regression subset selection, including exhaustive
search.
> leaps<-regsubsets(vol.ha
~age+si+ba.ha+stems.ha+topht+qdbh,data=standdat,nbest=10)
> # view results
> summary(leaps)
Subset selection object
Call: regsubsets.formula(vol.ha ~ age + si + ba.ha + stems.ha + topht +
   qdbh, data = standdat, nbest = 10)
6 Variables (and intercept)
        Forced in Forced out
           FALSE
                      FALSE
age
si
          FALSE FALSE
ba.ha FALSE FALSE
stems.ha FALSE FALSE
      FALSE FALSE
topht
qdbh
      FALSE
                 FALSE
10 subsets of each size up to 6
Selection Algorithm: exhaustive
```

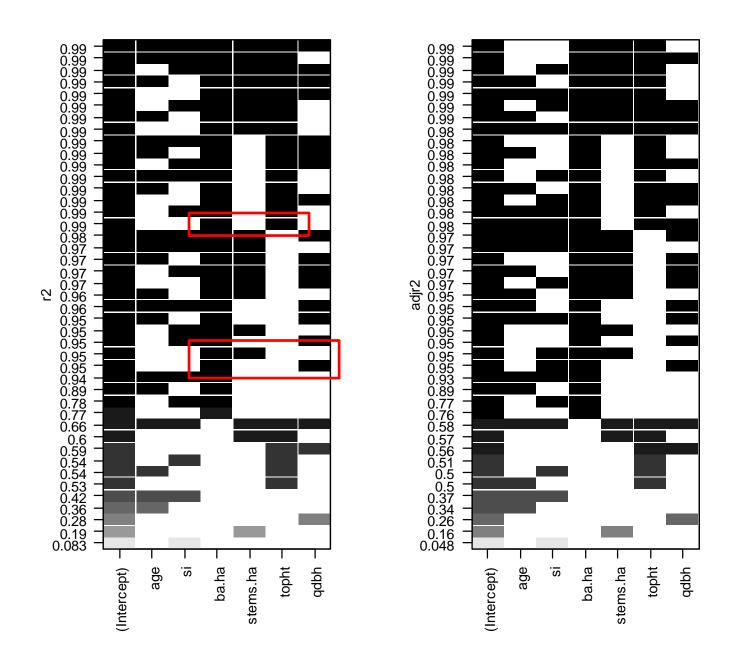
```
age si ba.ha stems.ha topht qdbh
         !!*!!!!!!!!!!!!!
                                     11 11
                                                   The best model with two predictors
         11 11 11 11 11 11 11 11 11 11
                                    11 11
                                                   contains stems.ha and topht
                                11 11 11 11
         11 11 11 11 11 11 11 11
                        11 * 11
         11 11 11 11 11 *11
                                     11 * 11
         "*" "*" "*" "*"
         11*11 11 11 11 11 11
         "*" "*" "*"
         || * || || * || || ||
```

Plot a table of models showing variables in each model.

- •This is particularly useful when there are more than ten models and the simple table produced by summary.regsubsets is too big to read.
- models are ordered by the selection statistic: "adjr2"or "r2"

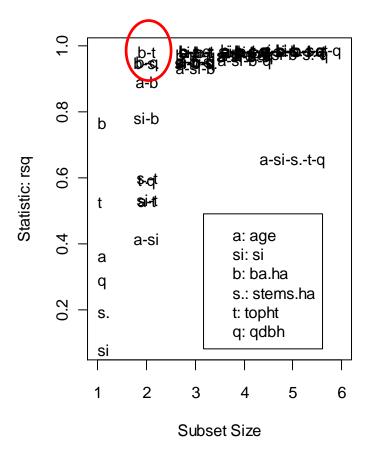
```
> par(mfrow=c(1,2),cex=0.7)
```

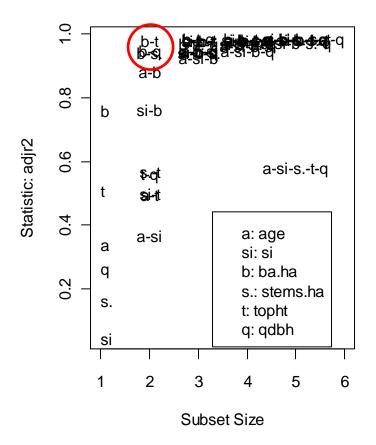
- > plot(leaps,scale="r2")
- > plot(leaps,scale="adjr2")
- > par(mfrow=c(1,1),cex=1)



Plot statistic by subset size

```
> library(car)
> par(mfrow=c(1,2))
> subsets(leaps, statistic="rsq")
> subsets(leaps, statistic="adjr2")
> par(mfrow=c(1,1))
```





For a number of models, select based on:

- Meeting assumptions: If an equation does not meet the assumption of a linear relationship, it is not a candidate model
- Compare the fit statistics. Select higher R² (or I²), and lower SE_F (or SE_F')
- Reject any models where the regression is not significant, since this model is no better than just using the mean of y as the predicted value.
- 4. Select a model that is biologically tractable. A simpler model is generally preferred, unless there are practical/biological reasons to select the more complex model
- 5. Consider the cost of using the model