

Statistics for the Sciences

Multiple Linear Regression Models

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Outline

- Introduction
- MLR Models
- Model formulation
- Scatter plot matrix
- Estimation
- ANOVA
- Statistical inferences
- Lab

Introduction

- loyn.csv: Loyn (1987) selected 56 forest patches in southeastern Victoria, Australia, and related the abundance of forest birds in each patch to six predictor variables: patch area (ha), distance to nearest patch (km), distance to nearest larger patch (km), grazing stock (1 to 5 indicating light to heavy), altitude (m) and years since isolation (years).

##	abund	area	yearisol	dist	distl	graze	alt
## 1	5.3	0.1	1968	39	39	2	160
## 2	2.0	0.5	1920	234	234	5	60
## 3	1.5	0.5	1900	104	311	5	140
## 4	17.1	1.0	1966	66	66	3	160
## 5	13.8	1.0	1918	246	246	5	140
## 6	14.1	1.0	1965	234	285	3	130
## 7	3.8	1.0	1955	467	467	5	90
## 8	2.2	1.0	1920	284	1829	5	60
## 9	3.3	1.0	1965	156	156	4	130
## 10	3.0	1.0	1900	311	571	5	130

Introduction

- Response variable abund, the target that we wish to predict
- with the following five **predictors** or independent variables as input
 - ▶ area
 - ▶ yearisol
 - ▶ dist
 - ▶ distl
 - ▶ graze
 - ▶ alt
- The aim was to develop a **best** predictive model relating bird abundance to these predictors. Perhaps we can use a model

$$\text{abund} \approx f(\text{area, dist, distl, graze, alt, yearisol})$$

Introduction

- We can refer to the input vector collectively as

$$X = \begin{pmatrix} X_1 \\ X_2 \\ X_3 \\ X_4 \\ X_5 \\ X_6 \end{pmatrix}$$

- Now we can write our model as

$$Y = f(X) + \varepsilon$$

where ε captures measurement errors and other discrepancies.

- ▶ One such model is Multiple Linear Regression Models

MLR Models

- Data:

Y	X_1	\dots	X_k
y_1	x_{11}	\dots	x_{1k}
\vdots	\vdots	\vdots	\vdots
y_n	x_{n1}	\dots	x_{nk}

- Y : Response variable
- X_1, X_2, \dots, X_k : Predictors or independent variables

MLR Models

Definition. A linear statistical model relating a random response Y to a set of independent variables X_1, X_2, \dots, X_k is of the form

$$Y|_{X_1=x_1, \dots, X_k=x_k} = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \dots + \beta_k x_k + \varepsilon,$$

where $\beta_0, \beta_1, \dots, \beta_k$ are unknown parameters, ε is a random variable, and the variables X_1, X_2, \dots, X_k assume known values.

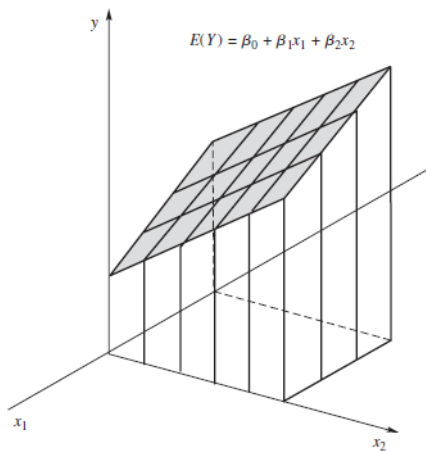
- We will assume that $E(\varepsilon) = 0$, and hence that

$$E(Y|_{X_1=x_1, \dots, X_k=x_k}) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \dots + \beta_k x_k.$$

- When $k = 1$, the model is the simple linear regression model.

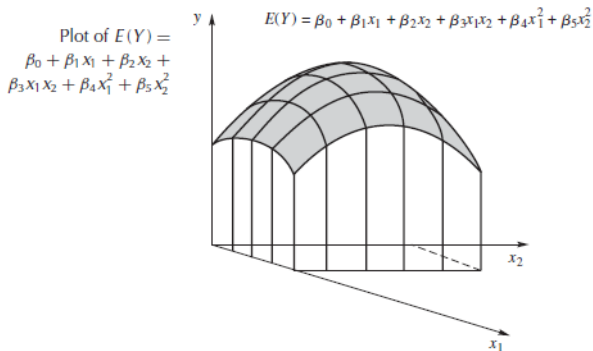
MLR Models

Plot of $E(Y) = \beta_0 + \beta_1 x_1 + \beta_2 x_2$



MLR Models

- **New predictors** can be created by transforming available predictors



MLR Models

- Matrix notation: We define the following matrices

$$\mathbf{Y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}, \quad \mathbf{X} = \begin{pmatrix} 1 & x_{11} & x_{12} & \cdots & x_{1k} \\ 1 & x_{21} & x_{22} & \cdots & x_{2k} \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & x_{n1} & x_{n2} & \cdots & x_{nk} \end{pmatrix}$$
$$\boldsymbol{\beta} = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_k \end{bmatrix}, \quad \boldsymbol{\varepsilon} = \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_n \end{bmatrix}$$

Then the MLR model can be written as

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon},$$

where $\boldsymbol{\varepsilon}$ has a multivariate distribution with mean $\mathbf{0}$ and variance-covariance matrix $\sigma^2 \mathbf{I}_n$, and \mathbf{I}_n is a n -dimensional identity matrix.

MLR Models

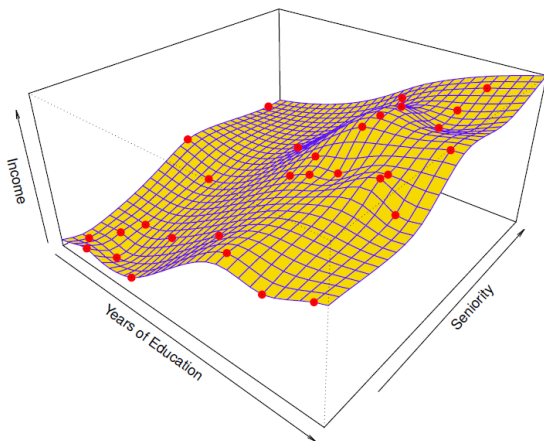
- \mathbf{Y} is generally assumed to have a multivariate normal distribution
 $\mathbf{Y} \sim MVN(\mathbf{X}\beta, \mathbf{\Sigma})$, where $\mathbf{\Sigma}$ is the Variance-Covariance Matrix of \mathbf{Y} :

$$\mathbf{\Sigma} = \begin{bmatrix} \text{Var}(Y_1) & \text{Cov}(Y_1, Y_2) & \cdots & \text{Cov}(Y_1, Y_n) \\ \text{Cov}(Y_2, Y_1) & \text{Var}(Y_2) & \cdots & \text{Cov}(Y_2, Y_n) \\ \vdots & \vdots & \ddots & \vdots \\ \text{Cov}(Y_n, Y_1) & \text{Cov}(Y_n, Y_2) & \cdots & \text{Var}(Y_n) \end{bmatrix} = \begin{bmatrix} \sigma^2 & 0 & \cdots & 0 \\ 0 & \sigma^2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \sigma^2 \end{bmatrix}$$

- **Question** What does linear in multiple linear regression models mean?

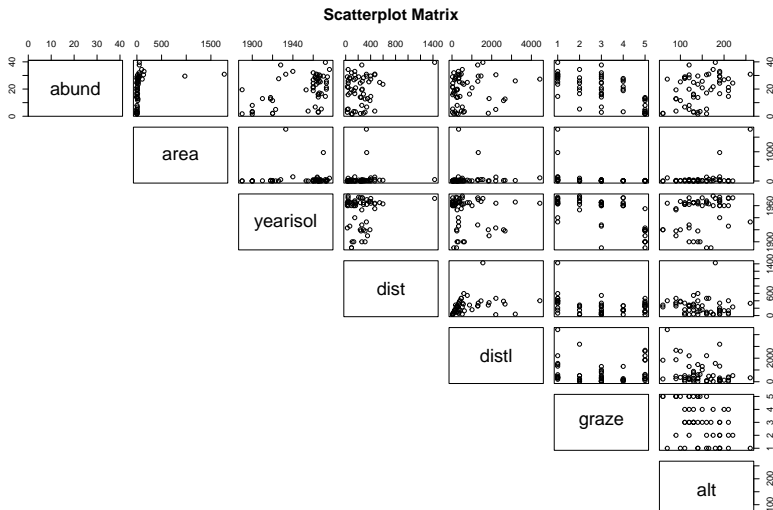
MLR Models

- We can build a very complex model without fitting errors (all fitted values are equal to the corresponding observed values). It is called **overfitting**.
 - ▶ Overfitting performs very bad in predictions.
 - ▶ It is often possible to get more accurate predictions with a simpler, instead of a complicated model.



Scatter plot matrix

- How do we build a reasonable **linear** model for given Y 's and predictors X_1, X_2, \dots, X_k ?
 - We need to check the relationship between Y and each X_i



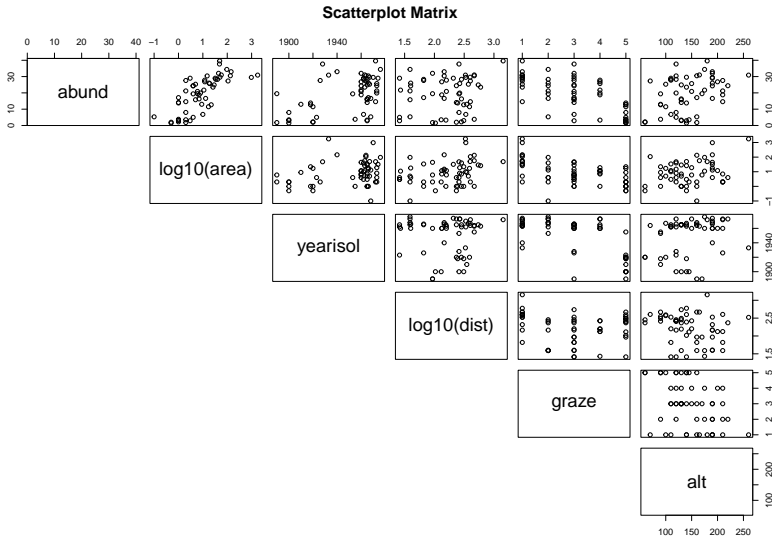
Scatter plot matrix

- We may check the correlation matrix as well

```
##          abund      area    yearisol      dist      distl      graze
## abund          1 0.2559702  0.503357741 0.2361125  0.08715258 -0.68251138
## area              1.0000000 -0.001494192 0.1083429  0.03458035 -0.31040242
## yearisol              1.000000000 0.1132175 -0.08331686 -0.63556710
## dist                  1.0000000  0.31717234 -0.25584182
## distl                  1.00000000  -0.02800944
## graze                      1.00000000
## alt
##          alt
## abund      0.3858362
## area       0.3877539
## yearisol   0.2327154
## dist       -0.1101125
## distl      -0.3060222
## graze      -0.4071671
## alt        1.0000000
```

Scatter plot matrix

- Now let's remove predictor `dist1` and consider log transformation of `area` and `dist`

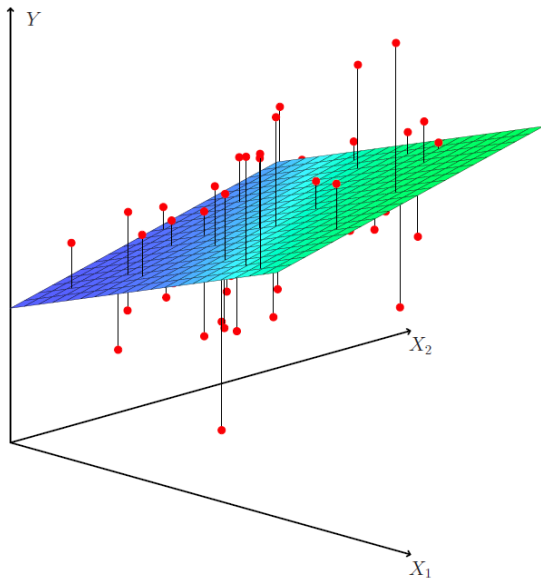


Scatter plot matrix

- The new correlation matrix

```
##          abund  logarea yearisol    logdist    graze      alt
## abund          1 0.7400358 0.5033577 0.12672333 -0.6825114 0.3858362
## logarea         1.0000000 0.2784145 0.30216662 -0.5590886 0.2751428
## yearisol         1.0000000 -0.01957223 -0.6355671 0.2327154
## logdist          1.00000000 -0.1426392 -0.2190070
## graze            1.0000000 -0.4071671
## alt              1.0000000
```


Estimation by Least Squares



Analysis of Variance

- The Analysis of Variance for MLR models can be summarized in the following table.

Source	df	SS	MS	F
Regression	k	SSR	$MSR = SSR/k$	MSR/MSE
Error	n-1-k	SSE	$MSE = SSE/(n-1-k)$	
Total	n-1	SS_{total}		

where $SSR = \sum_{i=1}^n (\hat{y}_i - \bar{y})^2$, $SSE = \sum_{i=1}^n (y_i - \hat{y}_i)^2$ and $SS_{total} = \sum_{i=1}^n (y_i - \bar{y})^2$.

- Note.** The F-test is for $H_0 : \beta_1 = \beta_2 = \dots = \beta_k = 0$ versus $H_a : \beta_i \neq 0$ for some $i = 1, 2, \dots, k$. And the F-test statistic (Exercise 11.84(a)) has an F distribution under H_0 with $df_1 = k$, $df_2 = n - 1 - k$.
- H_0 is rejected only if the calculated test statistic F^* is large: given significance level α , H_0 is rejected only if $F^* \geq F_{df_1, df_2, 1-\alpha}$.

Analysis of Variance

- The **Coefficient of Multiple Determination**, R^2 , is defined as

$$R^2 = \frac{SSR}{SST} = 1 - \frac{SSE}{SS_{total}}.$$

- R^2 is
 - ▶ The proportion of variation in the response explained by the regression.
 - ▶ The proportion by which the unexplained variation in the response is reduced by the regression.
- One problem with using R^2 to measure the quality of model fit, is that it can always be increased by adding another regressor.
- The **Adjusted Coefficient of Multiple Determination**, R_a^2 , is a measure that adjusts R^2 for the number of regressors in the model. It is defined as

$$R_a^2 = 1 - \frac{SSE/(n-1-k)}{SS_{total}/(n-1)}.$$

Statistical inference problems

- Suppose that the MLR model is

$$Y_i | X_1 = x_{1i}, \dots, X_k = x_{ki} = \beta_0 + \beta_1 x_{1i} + \beta_2 x_{2i} + \dots + \beta_k x_{ki} + \varepsilon_i, i = 1, \dots, k$$

- Inferences about individual parameters: $H_0 : \beta_i = 0$ versus $H_a : \beta_i \neq 0$, $i = 1, 2, \dots, k$
- Inferences about a set of parameters: testing $H_0 : \beta_{r+1} = \beta_{r+2} = \dots = \beta_k = 0$ versus H_a : At least one of the $\beta_i, i = r + 1, \dots, k$ differs from 0 which is checking if a reduced model is sufficient:
- Model R (Reduced model):

$$E(Y) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \dots + \beta_r x_r$$

- Model C (Complete model):

$$\begin{aligned} E(Y) = & \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \dots + \beta_r x_r \\ & + \beta_{r+1} x_{r+1} + \beta_{r+2} x_{r+2} + \dots + \beta_k x_k \end{aligned}$$

Statistical inference problems

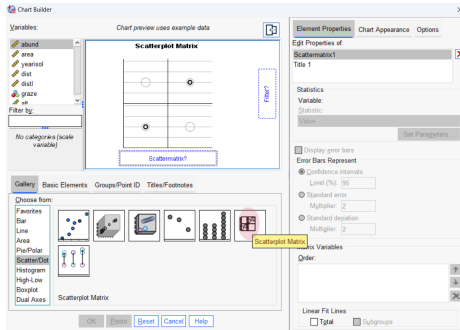
Let $\mathbf{x} = \mathbf{x}^* = (x_1^*, x_2^*, \dots, x_k^*)$ be a vector of new observation of the predictors.

- Predicting the average Value of Y : $E(Y) = \beta_0 + \beta_1 x_1^* + \beta_2 x_2^* + \dots + \beta_k x_k^*$
- Predicting a Particular Value of $Y = Y^* = \beta_0 + \beta_1 x_1^* + \beta_2 x_2^* + \dots + \beta_k x_k^* + \varepsilon$

Remark. Again, prediction intervals for the actual value of Y are longer than confidence intervals for $E(Y)$ if both confidence levels are the same and both are determined for the same value of $\mathbf{x} = \mathbf{x}^*$.

Lab

- loyn.csv: Loyn (1987) selected 56 forest patches in southeastern Victoria, Australia, and related the abundance of forest birds in each patch to six predictor variables: patch area (ha), distance to nearest patch (km), distance to nearest larger patch (km), grazing stock (1 to 5 indicating light to heavy), altitude (m) and years since isolation (years).
- After importing data, Click on Graphs in the top menu → Select Chart Builder... to plot a scatter plot matrix
 - ▶ In the Chart Builder dialog box, drag the Scatterplot Matrix under icon Scatter/Dot from the Gallery tab into the Chart Preview area.



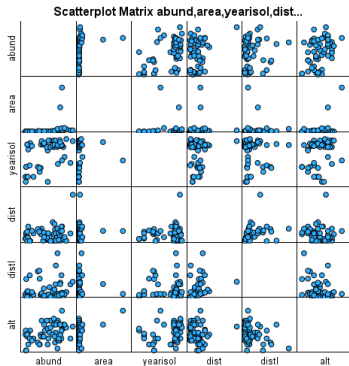
Lab

- Drag all numerical variables to the Scattermatrix? box.
 - graze is a nominal variable.

The screenshot shows the SPSS Chart Builder dialog box. On the left, the 'Variables:' list contains 'abund', 'area', 'yearisol', 'dist', 'distl', 'graze', and 'alt'. Below this is a 'Filter by:' section with a dropdown menu showing 'No categories (scale variable)'. The main area is titled 'Scatterplot Matrix abund,area,yearis...' and contains a preview of a 4x4 scatterplot matrix. A dashed box highlights the variables 'abund, area, yearisol, dist, distl, alt' in the preview. On the right, the 'Element Properties' tab is active, showing 'Edit Properties of: Scattermatrix1' and 'Title 1'. Below this, the 'Statistics' section is visible, with 'Variable:' set to 'Scattermatrix1' and 'Statistic:' set to 'Value'. The 'Error Bars Represent' section shows 'Confidence interval' selected with a level of 95%. The 'Matrix Variables' section shows 'Order:' set to 'abund', 'area', 'yearisol', 'dist'. The 'Linear Fit Lines' section has a checkbox for 'Total' which is unchecked. At the bottom, there are buttons for 'OK', 'Paste', 'Reset', 'Cancel', and 'Help'.

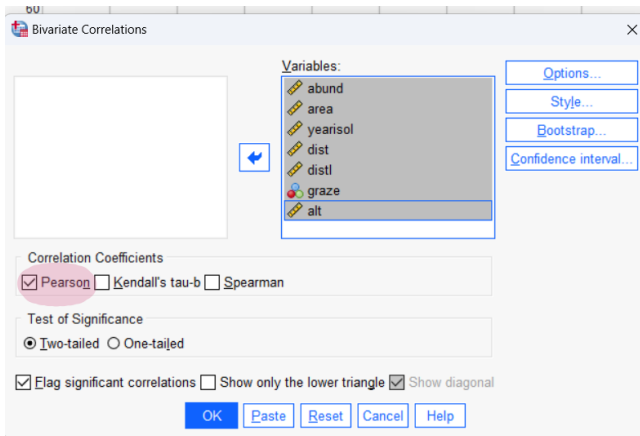
Lab

- Click OK to generate the scatter plot matrix.
- Or We can get a scatter plot matrix by clicking on Graphs → Scatter/Dot ... → Matrix Scatter



Lab

- To get the correlation matrix, click on Analyze → Correlate → Bivariate..., and then Add all numerical variables to the Variables box.



➔ **Correlations**

Correlations

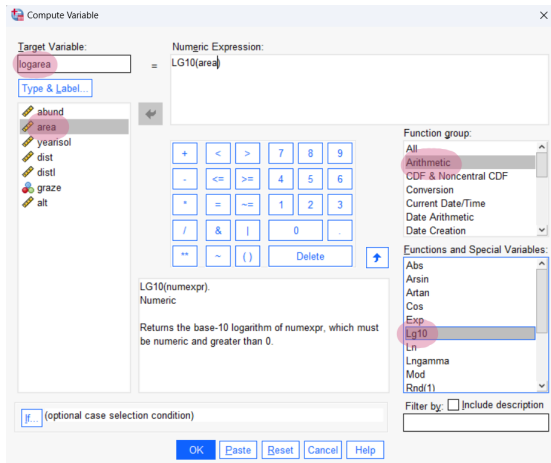
		abund	area	yearsol	dust	dustl	graze	alt
abund	Pearson Correlation	1	.256	.503**	.236	.087	-.683**	.386**
	Sig. (2-tailed)		.057	< .001	.080	.523	< .001	.003
	N	56	56	56	56	56	56	56
area	Pearson Correlation	.256	1	-.001	.108	.035	-.310*	.388**
	Sig. (2-tailed)	.057		.991	.427	.800	.020	.003
	N	56	56	56	56	56	56	56
yearsol	Pearson Correlation	.503**	-.001	1	.113	-.083	-.636**	.233
	Sig. (2-tailed)	< .001	.991		.406	.542	< .001	.084
	N	56	56	56	56	56	56	56
dust	Pearson Correlation	.236	.108	.113	1	.317*	-.256	-.110
	Sig. (2-tailed)	.080	.427	.406		.017	.057	.419
	N	56	56	56	56	56	56	56
dustl	Pearson Correlation	.087	.035	-.083	.317*	1	-.028	-.306*
	Sig. (2-tailed)	.523	.800	.542	.017		.838	.022
	N	56	56	56	56	56	56	56
graze	Pearson Correlation	-.683**	-.310*	-.636**	-.256	-.028	1	-.407**
	Sig. (2-tailed)	< .001	.020	< .001	.057	.838		.002
	N	56	56	56	56	56	56	56
alt	Pearson Correlation	.386**	.388**	.233	-.110	-.306*	-.407**	1
	Sig. (2-tailed)	.003	.003	.084	.419	.022	.002	
	N	56	56	56	56	56	56	56

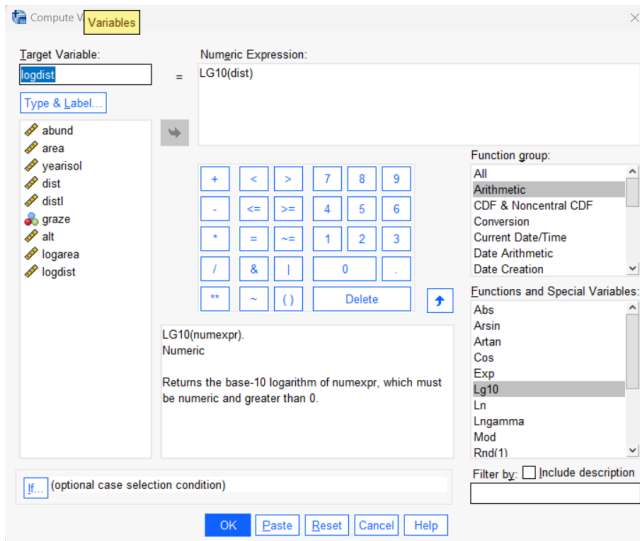
** . Correlation is significant at the 0.01 level (2-tailed).

* . Correlation is significant at the 0.05 level (2-tailed).

Lab

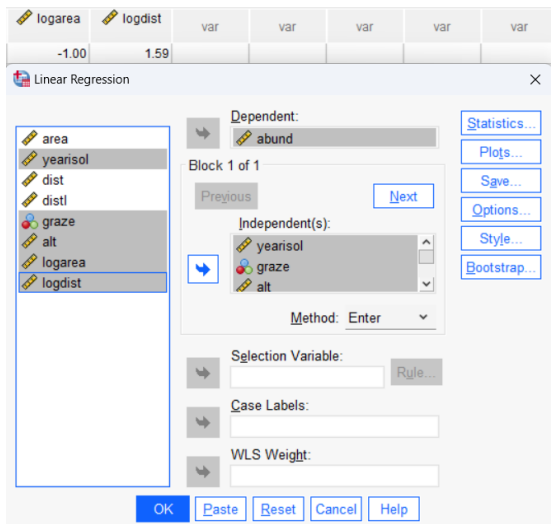
- Conduct log transformation for two variables area and dist
- Click on Transform → Compute Variable ...





Lab

- Follow the procedure fitting a simple linear regression model, to fit an MLR,
Click on Analyze → Regression → Linear ...
 - Model: $\text{abund} \sim \text{logarea} + \text{logdist} + \text{graze} + \text{alt} + \text{yearisol}$



Model Summary^b

Model	R	R Square	Adjusted R Square	Std. Error of the Estimate
1	.827 ^a	.684	.653	6.3256

a. Predictors: (Constant), logdist, yearisol, alt, logarea, graze

b. Dependent Variable: abund

ANOVA^a

Model		Sum of Squares	df	Mean Square	F	Sig.
1	Regression	4337.272	5	867.454	21.679	<.001 ^b
	Residual	2000.656	50	40.013		
	Total	6337.929	55			

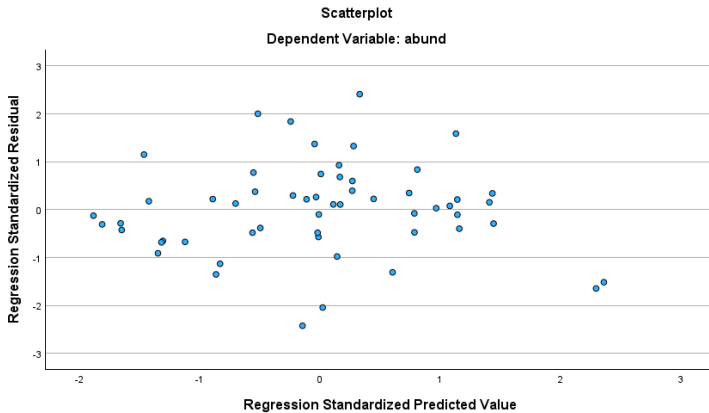
a. Dependent Variable: abund

b. Predictors: (Constant), logdist, yearisol, alt, logarea, graze

Coefficients^a

Model		Unstandardized Coefficients		Standardized Coefficients	t	Sig.	95.0% Confidence Interval for B	
		B	Std. Error	Beta			Lower Bound	Upper Bound
1	(Constant)	-131.847	88.640		-1.487	.143	-309.886	46.191
	yearisol	.077	.044	.182	1.744	.087	-.012	.165
	graze	-1.676	.921	-.230	-1.819	.075	-3.526	.174
	alt	.021	.023	.087	.937	.353	-.025	.067
	logarea	7.295	1.336	.552	5.460	<.001	4.612	9.979
	logdist	-1.303	2.319	-.050	-.562	.577	-5.961	3.354

a. Dependent Variable: abund



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