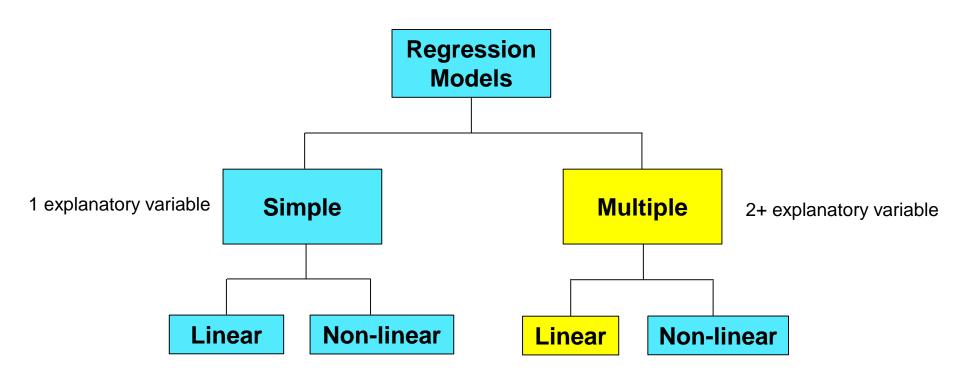
# Multiple regression and correlation

#### **Types of Regression Models**



# Regression modeling steps

#### 1. Hypothesize deterministic component

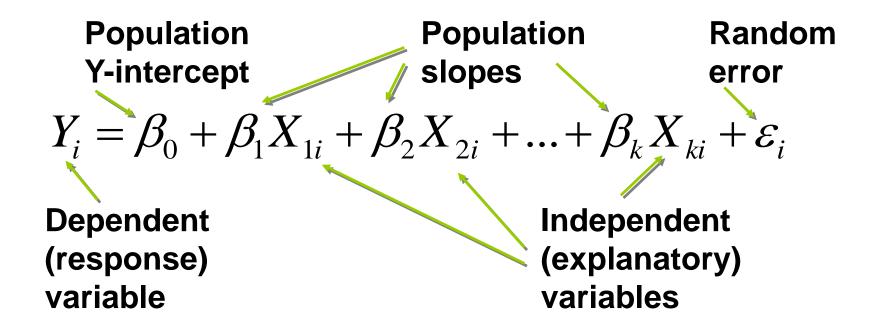
- 2. Estimate unknown model parameters
- 3. Specify probability distribution of random error term

estimate standard deviation of error

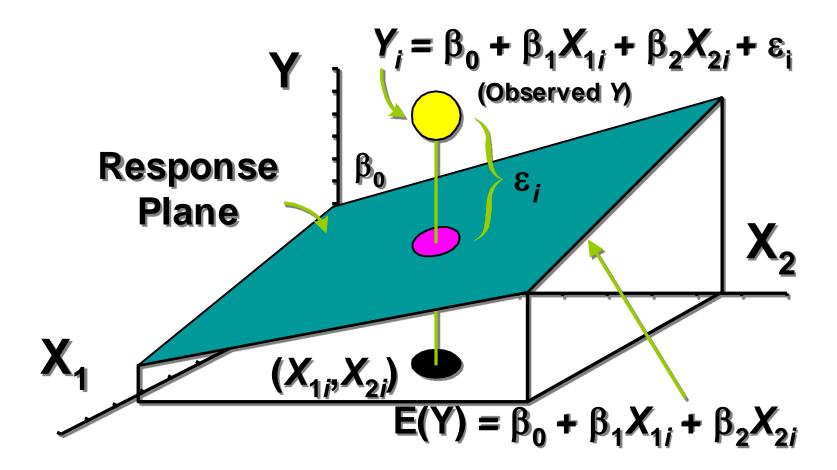
4. Evaluate model

# Linear multiple regression model

Relationship between 1 dependent & 2 or more independent variables is a linear function



## Bivariate regression model



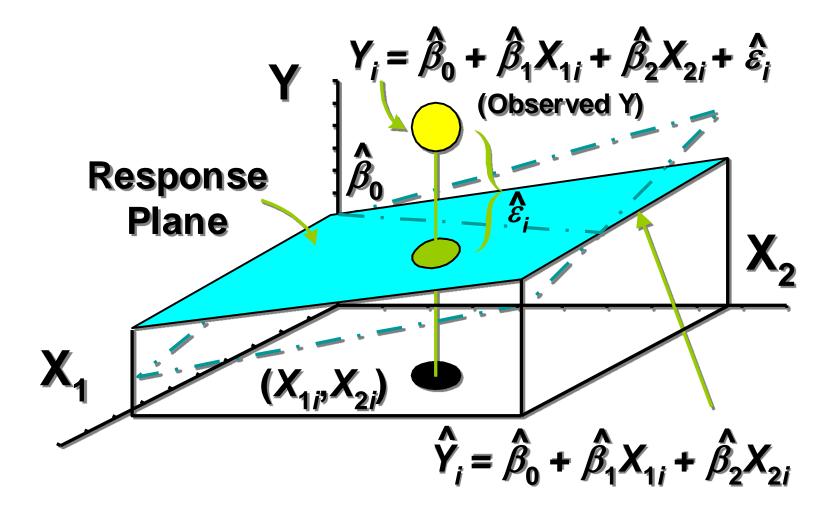
# Regression modeling steps

- 1. Hypothesize deterministic component
- 2. Estimate unknown model parameters
- 3. Specify probability distribution of random error term

Estimate standard deviation of error

4. Evaluate model

#### Estimate bivariate regression model



## Interpretation of estimated coefficients

- 1. Slope  $(\hat{\beta}_k)$ 
  - Estimated Y changes by  $\hat{\beta}_k$  for each 1 unit increase in  $x_k$  holding all other variables constant
    - Example: If  $\beta_1 \stackrel{\triangle}{=} 2$ , then sales (Y) is expected to increase by 2 for each 1 unit increase in advertising ( $X_1$ ) given the number of sales rep's ( $X_2$ )
- 2.Y-Intercept ( $\beta_0$ )
  - Average value of Y when  $X_k = 0$

#### Multiple regression in matrix

$$y_i = \beta_0 + \beta_1 x_{1i} + \beta_2 x_{2i} + \beta_3 x_{3i} + \varepsilon_i$$

$$\begin{pmatrix} y_{1} \\ y_{2} \\ y_{3} \\ \vdots \\ y_{n} \end{pmatrix} = \beta_{0} \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix} + \beta_{1} \begin{pmatrix} x_{11} \\ x_{12} \\ x_{13} \\ \vdots \\ x_{1n} \end{pmatrix} + \beta_{2} \begin{pmatrix} x_{21} \\ x_{22} \\ x_{23} \\ \vdots \\ x_{2n} \end{pmatrix} + \beta_{3} \begin{pmatrix} x_{31} \\ x_{32} \\ x_{33} \\ \vdots \\ x_{3n} \end{pmatrix} + \begin{pmatrix} \varepsilon_{1} \\ \varepsilon_{2} \\ \varepsilon_{3} \\ \vdots \\ \varepsilon_{n} \end{pmatrix}$$

$$= \begin{pmatrix} 1 & x_{11} & x_{21} & x_{31} \\ 1 & x_{12} & x_{22} & x_{32} \\ 1 & x_{13} & x_{23} & x_{33} \\ \vdots & \vdots & \vdots & \vdots \\ 1 & x_{1n} & x_{2n} & x_{3n} \end{pmatrix} \begin{pmatrix} \beta_{0} \\ \beta_{1} \\ \beta_{2} \\ \beta_{3} \end{pmatrix} + \begin{pmatrix} \varepsilon_{1} \\ \varepsilon_{2} \\ \varepsilon_{3} \\ \vdots \\ \varepsilon_{n} \end{pmatrix}$$

#### Least squares estimate (LSE)

The general multiple regression model is:

$$y = X \beta + \epsilon$$

$$\mathbf{X} = (X_1, X_2, \cdots X_p)$$

$$X_{i} = (X_{1i}, X_{2i}, \dots X_{ni})'$$
  $(i = 1 \text{ to } p)$ 

The LSE solution for  $\beta$  will be:

Min 
$$SSE = \sum_{i=1}^{n} (y_i - \beta_0 - \beta_1 X_{i1} - \dots - \beta_p X_p)^2$$
  $\hat{\beta}_1 = \frac{SS_{xy}}{SS_{xx}}$ 

In matrix notation:

$$X' y = X' X \hat{\beta} \implies \hat{\beta} = (X'X)^{-1}(X'y)$$

$$X'\mathbf{y} = \begin{pmatrix} \mathbf{1}'\mathbf{y} \\ X_1'\mathbf{y} \\ X_2'\mathbf{y} \\ X_3'\mathbf{y} \end{pmatrix} \qquad XX = SSCP = \begin{pmatrix} \mathbf{1}'\mathbf{1} & \mathbf{1}'X_1 & \cdots & \mathbf{1}'X_p \\ X_1'\mathbf{1} & X_1'X_1 & \cdots & X_1'X_p \\ X_2'\mathbf{1} & X_2'X_1 & \cdots & X_2'X_p \\ \vdots & \vdots & \ddots & \vdots \\ X_p'\mathbf{1} & X_p'X_1 & \cdots & X_p'X_p \end{pmatrix}$$

X' (X-prime or X-transpose)

#### Sum of squares and cross-products matrix (SSCP)

$$\mathbf{X} = \begin{bmatrix} a_1 & b_1 & c_1 \\ a_2 & b_2 & c_2 \\ a_3 & b_3 & c_3 \\ a_4 & b_4 & c_4 \end{bmatrix}$$

$$\mathbf{X} = \begin{bmatrix} a_1 & b_1 & c_1 \\ a_2 & b_2 & c_2 \\ a_3 & b_3 & c_3 \\ a_4 & b_4 & c_4 \end{bmatrix} \qquad \mathbf{X'} \mathbf{X} = \begin{bmatrix} a_1 & a_2 & a_3 & a_4 \\ b_1 & b_2 & b_3 & b_4 \\ c_1 & c_2 & c_3 & c_4 \end{bmatrix} \begin{bmatrix} a_1 & b_1 & c_1 \\ a_2 & b_2 & c_2 \\ a_3 & b_3 & c_3 \\ a_4 & b_4 & c_4 \end{bmatrix}$$

$$\mathsf{SSCP} = \mathsf{X'} \; \mathsf{X=} \begin{bmatrix} \sum a_i^2 & \sum a_i b_i & \sum a_i c_i \\ \sum b_i a_i & \sum b_i^2 & \sum b_i c_i \\ \sum c_i a_i & \sum c_i b_i & \sum c_i^2 \end{bmatrix}$$

# Correlation matrix and variance-covariance matrix

A <- matrix(c(1,2,2,3,2,2,2,3,4,3,4,2,0,2,2,2,0,0),6,3); A SSCP <- t(A) %\*% A; SSCP

cor(A) # correlation matrix 1.00 0.35 0.58 0.35 1.00 0.41 0.58 0.41 1.00

A.dev = A - rep(apply(A, 2, mean), each = length(A[,1])) # deviance t(A.dev) %\*% A.dev / (length(A[,1])-1) # variance-covariance matrix var(A) # variance-covariance matrix

library(MASS)
ginv(SSCP) # inverse matrix
ginv(ginv(SSCP)); SSCP
ginv(A) %\*% A

1	2	0
2	3	2
2	4	2
3	3	2
2	4	0
2	2	0

26	37	14
37	58	20
14	20	12

- 1	-1	- 1
0	0	1
0	1	1
1	0	1
0	1	-1

0.4	0.2	0.4
0.2	8.0	0.4
0.4	0.4	1.2

1	0	0
0	1	0
0	0	1

#### Fitted value and residual

The fitted value of  $\mathbf{y}$ , denoted  $\hat{\mathbf{y}}$ , is:

$$\hat{\mathbf{y}}_{n\times 1} = \mathbf{X}\hat{\boldsymbol{\beta}}$$

and the residual terms:

$$\underset{n\times 1}{e}=y-\hat{y}=y-X\hat{\beta}$$

we estimate residual  $\sigma^2$  from sample:

$$\mathbf{s}^2(e) = MSE$$

# Confidence intervals and tests of hypotheses for $\beta$

One - tailed test

$$H_0: \beta_i = 0$$

$$H_0: \beta_i = 0$$

$$H_a: \beta_i > 0 \text{ or } (\beta_i < 0)$$

$$H_a: \beta_i \neq 0$$

test statistic: 
$$t = \frac{\hat{\beta}_i}{s\sqrt{c_{ii}}}$$

Rejection region:

$$t > t_a \text{ (or } t < t_a)$$

$$|t| > t_{\alpha/2}$$

 $t_{\alpha/2}$  is based on [n - (p+1)]df, p is number of independent variables in the model

Page 425 (Zar, 1999)

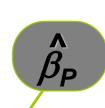
## Parameter estimation example

The abundance (Abund) of Tibetan wild ass is associated with habitat features such as grass coverage (Cover) and elevation (Elev). We want to find the effect of these two variables.

#### **Data**

	Abund	Cover	Elev
[1,]	41	80	4835
[2,]	22	48	3216
[3,]	31	40	5012
[4,]	9	24	2818
[5 <b>,</b> ]	39	64	5201
[6,]	11	8	3678

#### Parameter estimation



Abund = c(41, 22, 31, 9, 39, 11) Cover = c(80, 48, 40, 24, 64, 8) Elev = c(4835, 3216, 5012, 2818, 5201, 3678) fit = Im(Abund ~ Cover + Elev)

fit = Im(Abund ~ Cover + Elev)
summary(fit)

#### Coefficients:

```
t value Pr(>|t|)
                         Std. Error
             Estimate
(Intercept)
                        2.395e+00
                                     -7.035
                                             0.00590
            -1.685e+01
             3.144e-01
                        2.715e-02
                                     11.581
                                             0.00138
                                                      **
Cover
                        6.977e-04
             6.911e-03
                                             0.00219
                                                      **
Elev
                                      9.905
                               '**' 0.01
Signif.
        codes:
                         0.001
                                         '*' 0.05 '.'
0.1
```

#### Interpretation of coefficients solution

# 1. Slope $(\hat{\beta}_1)$

 Responses to Cover is expected to increase by 0.31 individual for each 1 percent of increase in grass coverage holding elevation constant

# 2. Slope $(\hat{\beta}_2)$

 Responses to Elev is expected to increase by 0.0069 individual for each 1 meter increase in elevation holding coverage constant

#### Regression modeling steps

- 1. Hypothesize deterministic component
- 2. Estimate unknown model parameters
- 3. Specify probability distribution of random error term

Estimate standard deviation of error

4. Evaluate model

#### Variance of error

Best (unbiased) estimator of  $\sigma^2 = Var(\varepsilon)$ 

is

$$S^{2} = \frac{SSE}{n - (k+1)} = \frac{\sum \hat{\varepsilon}_{i}^{2}}{n - (k+1)}$$

Variance of error is used in formula for computing parameter SD (standard deviation)

$$S_{\hat{\beta}_i} = S\sqrt{C_{ii}}$$

Parameter distribution:

$$t = \frac{\hat{\beta}_i}{S\sqrt{C_{ii}}}$$

## Regression modeling steps

- 1. Hypothesize deterministic component
- 2. Estimate unknown model parameters
- Specify probability distribution of random error term

Estimate standard deviation of error

#### 4. Evaluate model

# Evaluating multiple regression model steps

- 1. Examine variation measures
- 2. Do residual analysis
- 3. Test parameter significance

Overall model

Individual coefficients

4. Test for multicollinearity

## **Basic assumptions**

- Mean value of the outcome variable for a set of explanatory variables is described by the regression equation.
- Normal distribution of values around the regression line.
- Variance around the regression line is the same for all values of the explanatory variables.
- The explanatory variables are not correlated.

## Multiple coefficient of determination

• The  $R^2$  statistic measures the overall contribution of Xs.

$$R^2 = \frac{\text{Explained variation}}{\text{Total variation}} = \frac{SS_y - SSE}{SS_y} = 1 - \frac{SSE}{SS_y}$$

# Adjusted R<sup>2</sup>

- R<sup>2</sup> never decreases when new variable is added to model
  - disadvantage when comparing models
- Solution: Adjusted R<sup>2</sup>
  - Each additional variable reduces adjusted R<sup>2</sup>

$$R_a^2 = 1 - \left[\frac{n-1}{n-(k+1)}\right] \frac{SSE}{SS_y} \le 1 - \frac{SSE}{SS_y} = R^2$$

# Evaluating multiple regression model steps

- 1. Examine variation measures
- 2. Do residual analysis
- 3. Test parameter significance
  - Overall model
  - Individual coefficients
- 4. Test for multicollinearity

## Residual analysis

- 1. Graphical analysis of residuals
  - Plot estimated errors vs.  $X_i$  values
  - Plot histogram or scatter of residuals

#### 2. Purposes

- Examine functional form (linear vs. non-linear model)
- Evaluate violations of assumptions

#### Assumptions for residuals/errors

- 1. Mean of probability distribution of error is 0
- 2. Probability distribution of error has constant variance
- 3. Probability distribution of error is normal
- 4. Errors are independent

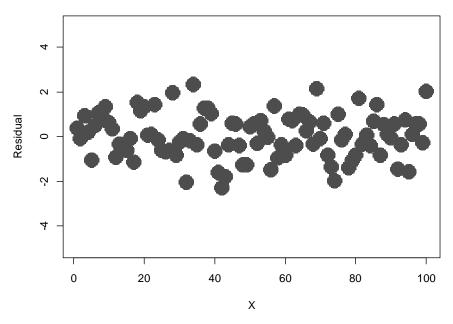
#### Residual plot for functional form



# Residual Note that the serious of t

#### X = 1:100; Y = -(X-50)^2 + rnorm(100, 1000, 500) plot(X, Y, cex=3, xlab='X', ylab='Residual', pch=16, col='gray30')

#### **Correct Specification**

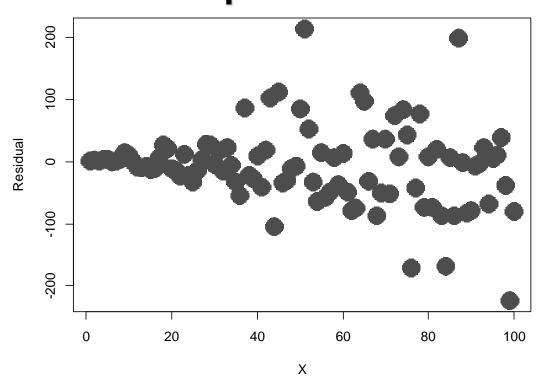


X = 1:100; Y = rnorm(100, 0, 1) plot(X, Y, ylim=c(-5,5), cex=3, xlab='X', ylab='Residual', pch=16, col='gray30')

## Residual plot for equal variance



#### **Unequal Variance**

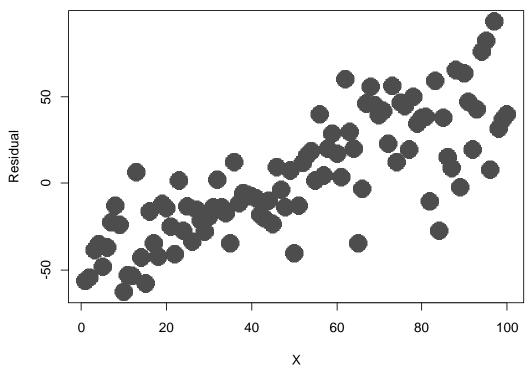


Fan-shaped

## Residual plot for independence



#### **Not Independent**



#### Checking independence and linearity

library(car)

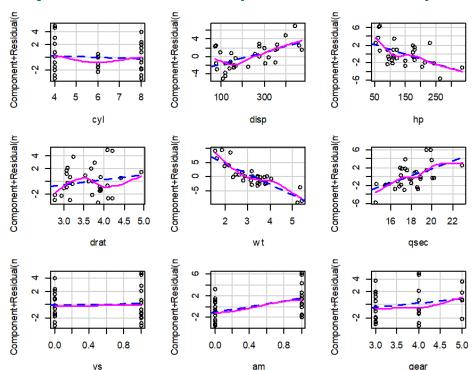
fit =  $lm(mpg \sim ., data=mtcars)$ 

durbinWatsonTest(fit) #Durbin-Watson Test for Autocorrelated Errors

lag Autocorrelation D-W Statistic p-value 1 0.03101277 1.860893 0.342

Alternative hypothesis: rho != 0

#### crPlots(fit) #Component+Residual (Partial Residual) Plots



# Evaluating multiple regression model steps

- 1. Examine variation measures
- 2.Do residual analysis
- 3. Test parameter significance
  - Overall model
  - Individual coefficients
- 4. Test for multicollinearity

## Testing overall significance

- 1.Shows if there is a linear relationship between **all** *X* variables **together** & *Y*
- 2.Uses F test statistic (SSR vs. SSE)
- 3. Hypotheses

$$- H_0$$
:  $\beta_1 = \beta_2 = ... = \beta_k = 0$ 

- No Linear Relationship
- H<sub>a</sub>: At least one coefficient is not 0
  - At least one X variable affects Y

#### F Statistic for model significance

$$F = \frac{MSR}{MSE} = \frac{SSR/k}{SSE/(n-k-1)}$$

$$F = \frac{R^2 / k}{(1 - R^2) / (n - k - 1)}$$

Rejection region:  $F_{v1,v2} > F_a$ , where  $v_1 = k$ ,  $v_2 = n - (k+1)$ 

Now the collective contribution of Xs can be evaluated.

#### Model and parameter significance

model = Im(log(trees\$Volume)~log(trees\$Girth)+log(trees\$Height))
summary(model)

```
Coefficients:
                Estimate
                         Std. Error t value
                                                Pr(>|t|)
(Intercept)
                -6.63162 0.79979
                                       -8.292
                                                5.06e-09 ***
log(trees$Girth)
                                       26.432
                                                < 2e-16 ***
                1.98265
                          0.07501
log(trees$Height) 1.11712
                          0.20444
                                       5.464
                                                7.81e-06 ***
Residual standard error: 0.08139 on 28 degrees of freedom Multiple
R-squared: 0.9777, Adjusted R-squared: 0.9761 F-statistic: 613.2 on
2 and 28 DF, p-value: < 2.2e-16
```

# Evaluating multiple regression model steps

- 1. Examine variation measures
- 2. Do residual analysis
- 3. Test parameter significance
  - Overall model
  - Individual coefficients

#### 4. Test for multicollinearity

## Multicollinearity

- High correlation between X variables
- Leads to unstable coefficients depending on X variables in model
- Always exists -- matter of degree
- Example: using both age & height as explanatory variables for weight

#### **Detecting multicollinearity**

#### Examine correlation matrix

correlations between pairs of X variables are more than with Y variable

Examine variance inflation factor (VIF)

$$VIF_j = \frac{1}{1 - R_i^2}$$

 $R_j^2$  is the multiple correlation coefficient, the coefficient of determination of:

$$X_{j} = \beta_{0} + \beta_{1}X_{1} + \ldots + \beta_{j-1}X_{j-1} + \beta_{j+1}X_{j+1} + \ldots + \beta_{k}X_{k} + \varepsilon$$

If VIF<sub>i</sub> > 5 (or 10 according to text), multicollinearity exists.

#### Interpretation

The square root of the variance inflation factor tells you how much larger the standard error is, compared with what it would be if that variable were uncorrelated with the other independent variables in the equation.

#### **Example**

If the variance inflation factor of an independent variable were 5.27 ( $\sqrt{5.27}$  = 2.3) this means that the standard error for the coefficient of that independent variable is 2.3 times as large as it would be if that independent variable were uncorrelated with the other independent variables.

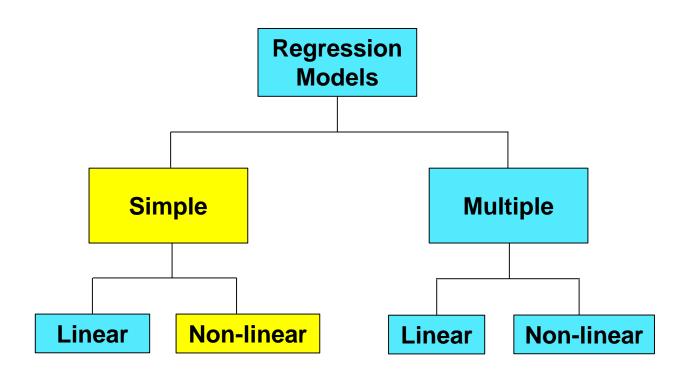
## R code - VIF (variance inflation factor)

```
library(car)
vif(lm(mpg ~ ., data = mtcars))
```

cyl	disp	hp	drat	wt	qsec	VS	am	gear	carb
15.37	21.62	9.83	3.37	15.16	7.53	4.97	4.65	5.36	7.91

	mpg	cyl	disp	hp	drat	wt	qsec	VS	am	gear	carb
Mazda RX4	21.0	6	160.0	110	3.90	2.620	16.46	0	1	4	4
Mazda RX4 Wag	21.0	6	160.0	110	3.90	2.875	17.02	0	1	4	4
Datsun 710	22.8	4	108.0	93	3.85	2.320	18.61	1	1	4	1
<b>Hornet 4 Drive</b>	21.4	6	258.0	110	3.08	3.215	19.44	1	0	3	1
<b>Hornet Sportabout</b>	18.7	8	360.0	175	3.15	3.440	17.02	0	0	3	2
Valiant	18.1	6	225.0	105	2.76	3.460	20.22	1	0	3	1

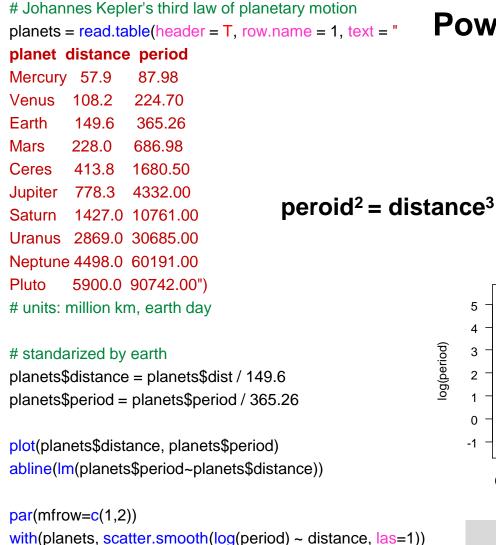
### **Types of Regression Models**



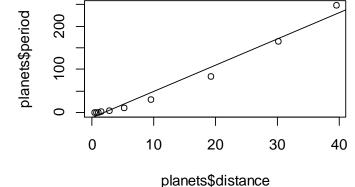


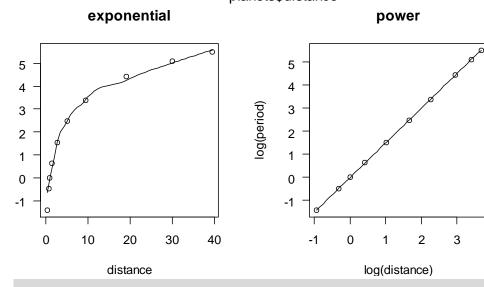
Biostatistics Xinhai Li

Lecture 12. Multiple regression and correlation



### Power function





Estimate Std. Error t value Pr(>|t|)
(Intercept) -0.0000667 0.0004349 -0.153 0.882
log(distance) 1.5002315 0.0002077 7222.818 <2e-16 \*\*\*

Residual standard error: 0.001016 on 8 degrees of freedom

Multiple R-squared: 1, Adjusted R-squared: 1 F-statistic: 5.217e+07 on 1 and 8 DF, p-value: < 2.2e-16

summary(lm(log(period) ~ log(distance), data=planets))

with(planets, scatter.smooth(log(period) ~ log(distance), las=1))

title(main="exponential")

title(main="power")

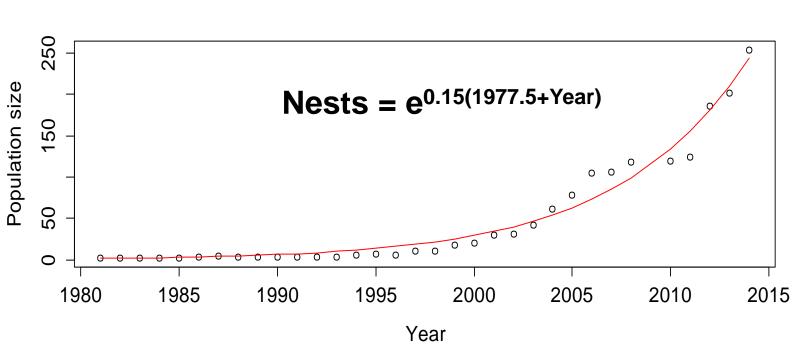
41

Year

Xinhai Li

Nests

# **Exponential function**



```
1982
1983
1984
1985
1986
1987
1988
1989
1990
1991
1992
1993
1994
1995
1996
1997
            11
1998
            11
1999
            18
2000
            20
2001
            30
2002
            31
2003
2004
            62
2005
            78
2006
           105
2007
           106
2008
           118
2010
           119
2011
           124
2012
           186
2013
           201
2014
```

```
out = n (Nest ~ exp(b1*(b0+Year)),
     data=D, start=list(b0=-1981, b1=1),
     trace = TRUE)
plot(D$Year, D$Nests)
lines(D$Year, fitted(out), col=2)
```

model: Nests ~ exp(b1 \* (b0 + Year)) data: D b0 = -1977.5; b1 = 0.15residual sum-of-squares: 4279

3

D\$time,

**D**\$plant

D\$weight,

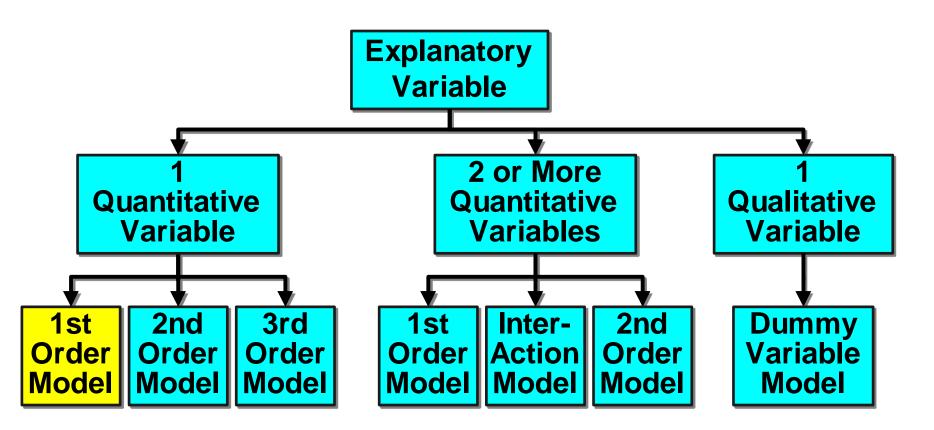
title(main="Graph of weight vs time")

#### # Logistic growth **Logistic function** time <- c(seq(0,10),seq(0,10),seq(0,10)) plant <- c(rep(1,11),rep(2,11),rep(3,11)) weight <- c( 42,51,59,64,76,93,106,125,149,171,199, 40,49,58,72,84,103,122,138,162,187,209, 41,49,57,71,89,112,146,174,218,250,288)/288 D <- data.frame(cbind(time, plant, weight)) ## Plot weight versus time plot( D\$time, 3 0.8 D\$weight, 3 xlab="Time", 9.0 ylab="weight", 0.4 type="n" 0.2 0 2 6 8 10 text(

Time

```
IN = getInitial(
 weight ~ SSlogis(time, alpha, xmid, scale),
 data = D
## Using the initial parameters above,
## fit the data with a logistic curve.
para0.st <- c(
 alpha = IN[1],
         = IN[2]/IN[3], # beta is xmid/scale
 gamma= 1/IN[3] # gamma (or r) is 1/scale
names(para0.st) = c('alpha', 'beta', 'gamma')
fit0 <- nls(
 weight ~ alpha/(1+exp(beta-gamma*time)),
 D,
 start = para0.st,
 trace = T
curve(
 2.21/(1 + \exp(2.74 - 0.22*x)),
 from = time[1],
 to = time[11],
 add = TRUE
                                           43
```

# Types of regression models (polynomial)



# First-order model with 1 independent variable

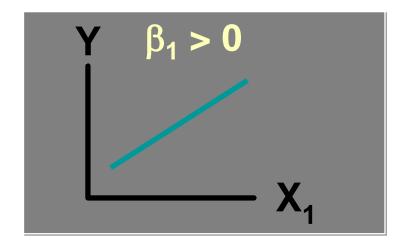
 Relationship between 1 dependent & 1 independent variable is linear

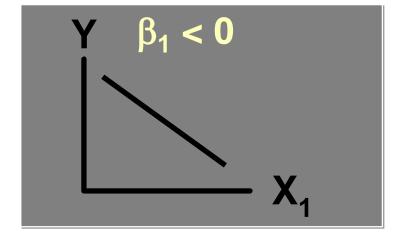
$$E(Y) = \beta_0 + \beta_1 X_{1i}$$

2. Used when expected rate of change in *Y* per unit change in *X* is stable

### First-order model relationships

$$E(Y) = \beta_0 + \beta_1 X_1$$



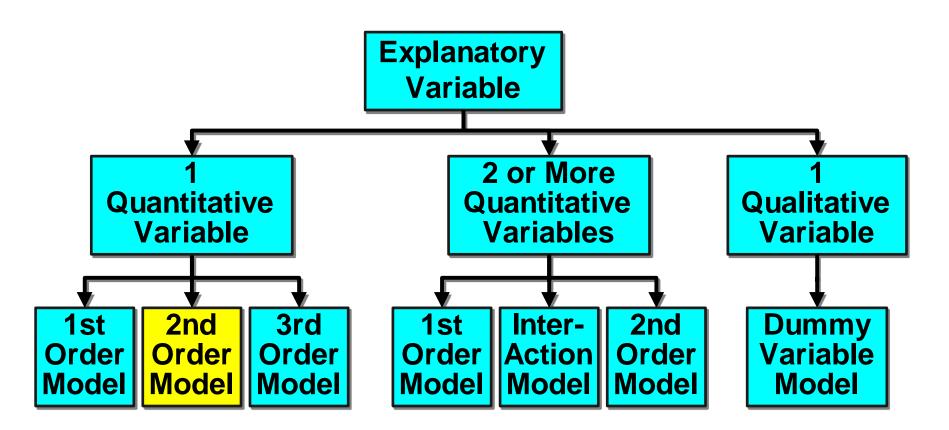


### First-order model worksheet

Case, i	Yi	<b>X</b> <sub>1i</sub>
1	1	1
2	4	8
3	1	3
4	3	5
;		;

Run regression with  $Y, X_1$ 

# Types of regression models (polynomial)

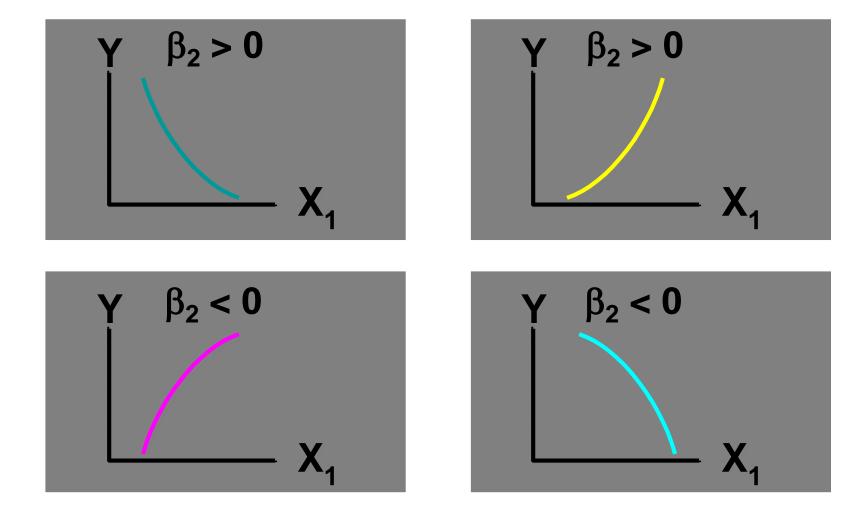


# Second-order model with 1 independent variable

- Relationship between 1 dependent & 1 independent variables is a quadratic function
- 2. Model:

Nodel: Curvilinear effect 
$$E(Y) = \beta_0 + \beta_1 X_1 + \beta_2 X_1^2$$
 Linear effect

### Second-order model relationships

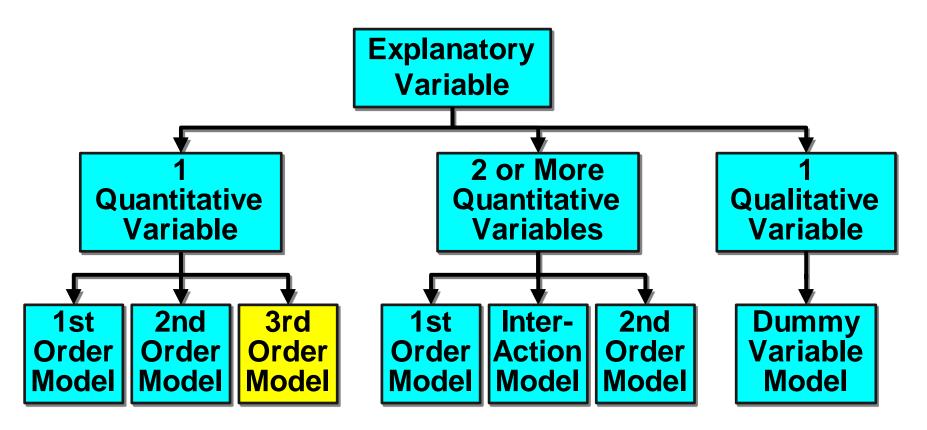


### Second-order model worksheet

Case, i	$Y_i$	$X_{1i}$	$X_{1i}^2$
1	1	1	1
2	4	8	64
3	1	3	9
4	3	5	25
:	;	•••	;

Create  $X_1^2$  column. Run linear regression with Y,  $X_1$ ,  $X_1^2$ .

# Types of regression models (polynomial)



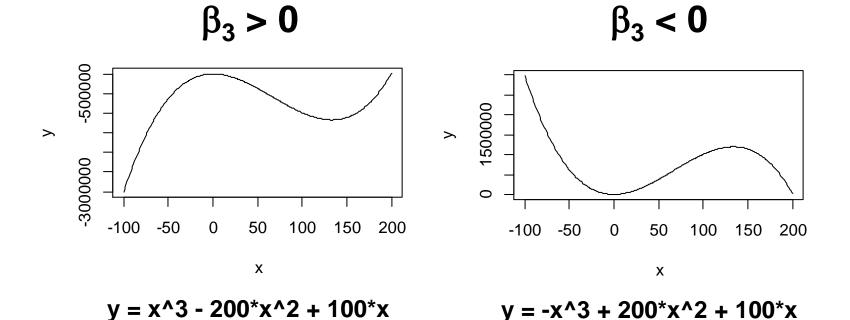
# Third-order model with 1 independent variable

- 1.Relationship between 1 dependent & 1 independent variable has a 'wave'
- 2.Used if 1 reversal in curvature
- 3.Model:

$$E(Y) = \beta_0 + \beta_1 X_1 + \beta_2 X_1^2 + \beta_3 X_1^3$$
 Linear effect Curvilinear effects

## Third-order model relationships

$$E(Y) = \beta_0 + \beta_1 X_1 + \beta_2 X_1^2 + \beta_3 X_1^3$$

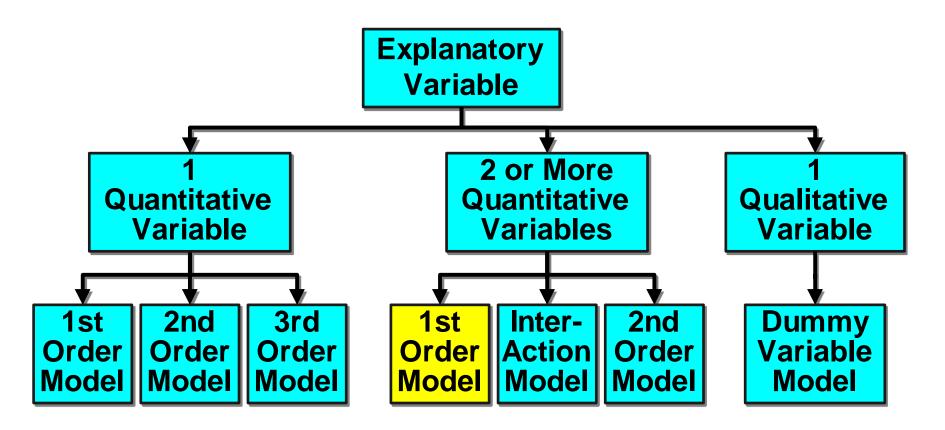


### Third-order model worksheet

Case, i	$Y_i$	<b>X</b> <sub>1i</sub>	$X_{1i}^2$	$X_{1i}^3$
1	1	1	1	1
2	4	8	64	512
3	1	3	9	27
4	3	5	25	125
;	:	;	;	;

Multiply  $X_1$  by  $X_1$  to get  $X_1^2$ Multiply  $X_1$  by  $X_1$  by  $X_1$  to get  $X_1^3$ Run regression with Y,  $X_1$ ,  $X_1^2$ ,  $X_1^3$ 

# Types of regression models (polynomial)

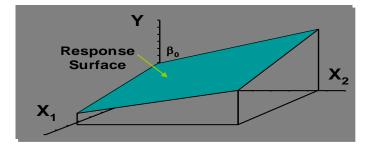


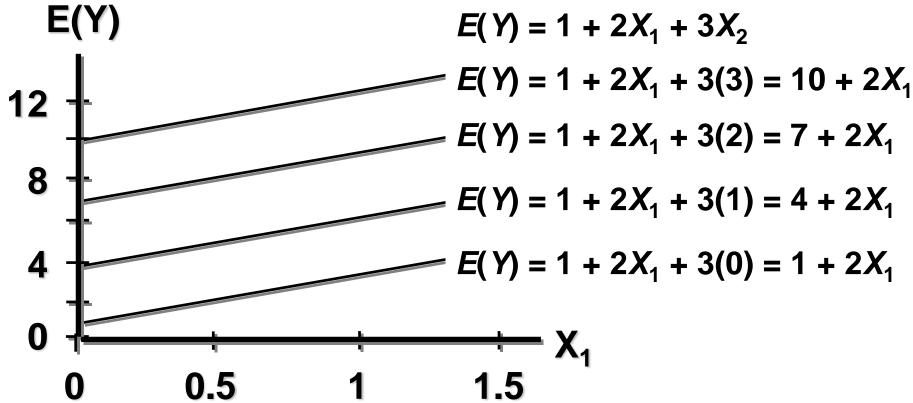
# First-order model with 2 independent variables

- 1.Relationship between 1 dependent &2 independent variables is a linear function
- 2. Assumes no interaction between  $X_1 \& X_2$ 
  - Effect of  $X_1$  on E(Y) is the same regardless of  $X_2$  values
- 3.Model

$$E(Y) = \beta_0 + \beta_1 X_1 + \beta_2 X_2$$

### No interaction





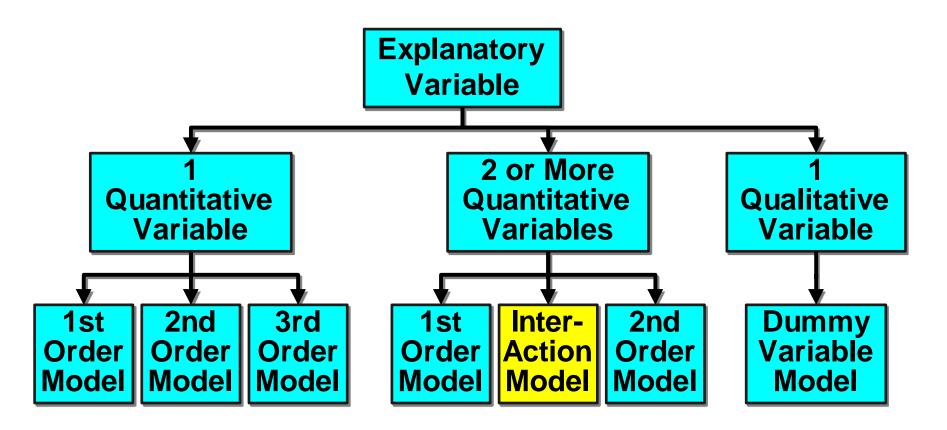
Effect (slope) of  $X_1$  on E(Y) does not depend on  $X_2$  value

### First-order model worksheet

Case, i	Yi	$X_{1i}$	X <sub>2i</sub>
1	1	1	3
2	4	8	5
3	1	3	2
4	3	5	6
**	**	***	**

Run regression with Y,  $X_1$ ,  $X_2$ 

# Types of regression models (polynomial)



# Interaction model with 2 independent variables

1. Hypothesizes interaction between pairs of *X* variables

Response to one *X* variable varies at different levels of another *X* variable

2. Contains two-way cross product terms

$$E(Y) = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_1 X_2$$

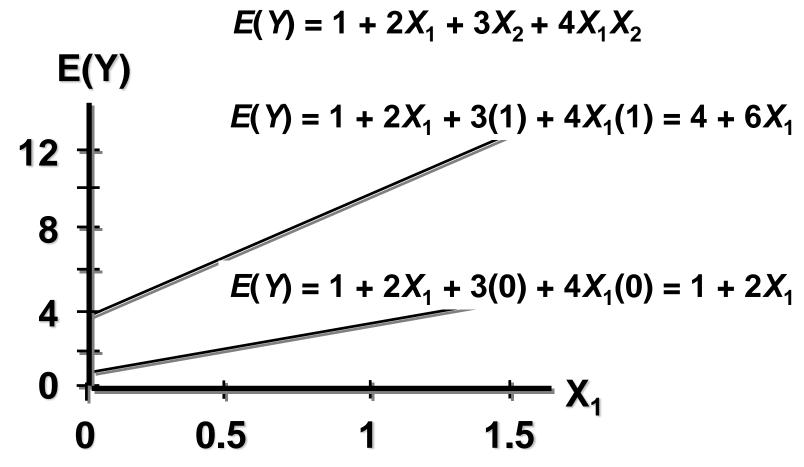
### **Effect of interaction**

1.Given:

$$E(Y) = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_1 X_2$$

- 2.Without interaction term, effect of  $X_1$  on Y is measured by  $\beta_1$
- 3.With interaction term, effect of  $X_1$  on Y is measured by  $\beta_1 + \beta_3 X_2$ 
  - Effect increases as  $X_{2i}$  increases

### Interaction model relationships



Effect (slope) of  $X_1$  on E(Y) does depend on  $X_2$  value

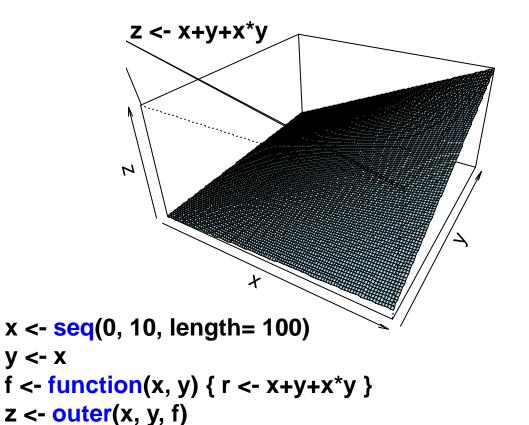
### Interaction model worksheet

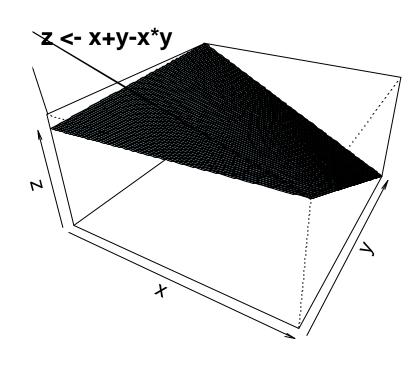
Case, i	$Y_i$	<b>X</b> <sub>1i</sub>	$X_{2i}$	$X_{1i} X_{2i}$
1	1	1	3	3
2	4	8	5	40
3	1	3	2	6
4	3	5	6	30
:	;		;	;

Multiply  $X_1$  by  $X_2$  to get  $X_1X_2$ . Run regression with Y,  $X_1$ ,  $X_2$ ,  $X_1X_2$ 

y <- x

#### Perspective plots for interaction models

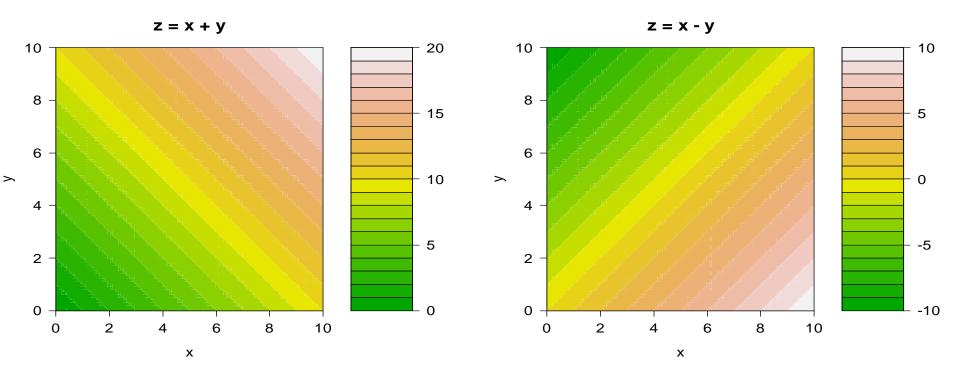




```
op <- par(bg = "white", mfrow=c(1,2))
persp(x, y, z, theta = 30, phi = 30, expand = 0.5,
      col = "lightblue", main='z=x+y+x*y')
```

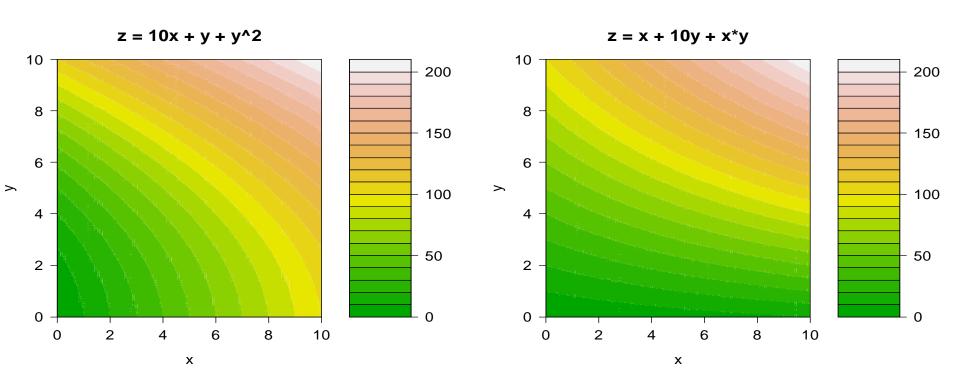
### Contour plots for models with linear terms

 $x = y \leftarrow seq(0, 10, length = 100); f \leftarrow function(x, y) \{ r \leftarrow x+y \}; z \leftarrow outer(x, y, f)$ filled.contour(x, y, z, main="z = x + y", color = terrain.colors)



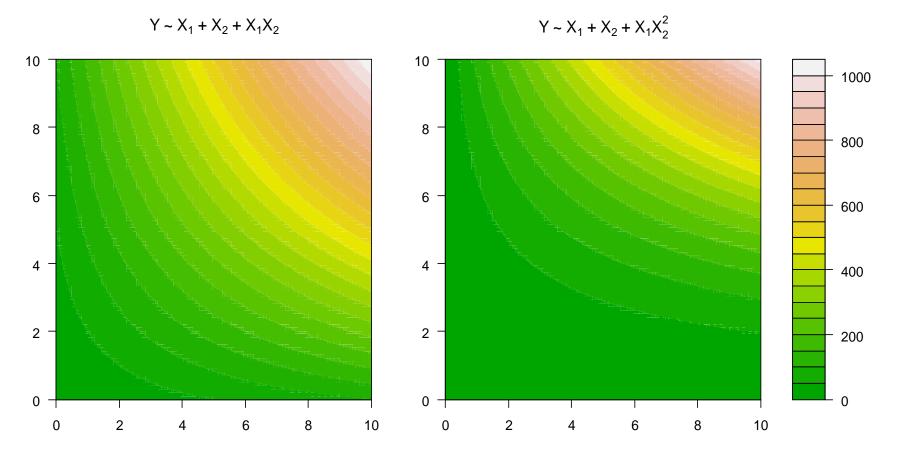
### Contour plots for high order models

filled.contour(x, y, z, main=z = x + 10y + xy, color = terrain.colors)



#### Contour plots for interaction models

 $x1 = x2 \leftarrow seq(0, 10, length = 100); f \leftarrow function(x1, x2) \{ r \leftarrow x1+x2+x1*x2*x2 \}; y \leftarrow outer(x1, x2, f)$  filled.contour(x1, x2, y, main=expression(paste("Y ~ ", X[1], " + ", X[2], " + ", X[1], X[2]^2)), color = terrain.colors) # [] subscript; ^ superscript



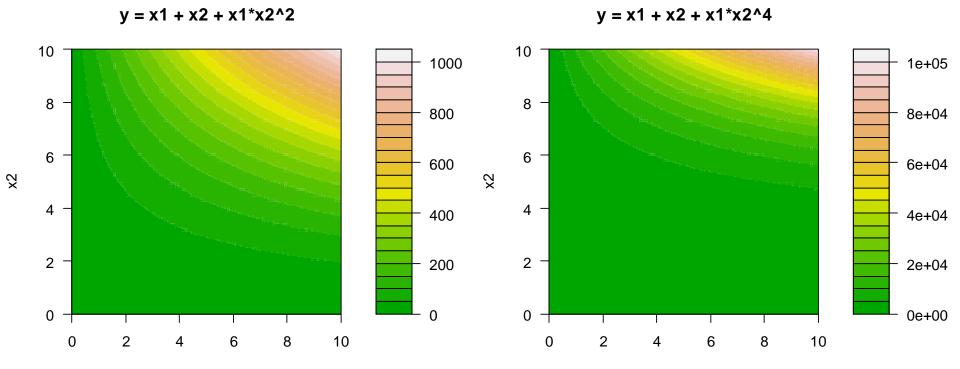
#### **Estimating regression coefficients**

x1 = 0.8485 x2 = 1.0099 x1:x2 = 0.9787

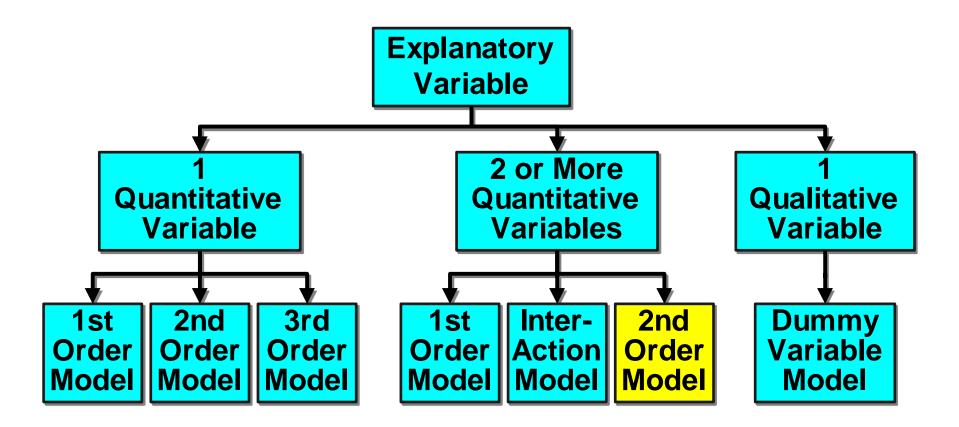
**x**1

x1 = 0.8198 x2 = 1.0145 x1:x2 = 0.7744

**x**1



## Types of regression models (detailed)



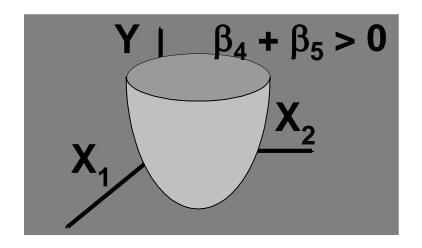
# Second-order model with 2 independent variables

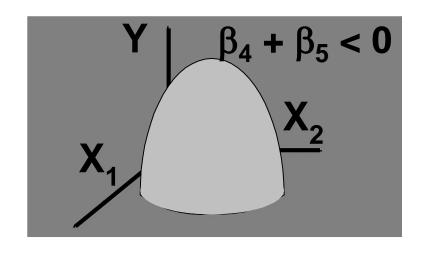
 Relationship between 1 dependent & 2 or more independent variables is a quadratic function

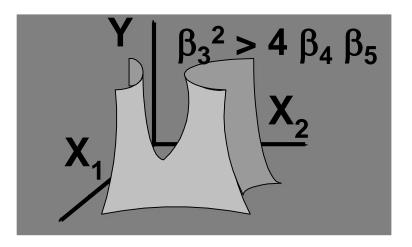
#### 2. Use model:

$$E(Y) = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_1 X_2 + \beta_4 X_1^2 + \beta_5 X_2^2$$

### Second-order model relationships







$$E(Y) = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_1 X_2 + \beta_4 X_1^2 + \beta_5 X_2^2$$

### Second-order model worksheet

Case, i	$Y_i$	<i>X</i> <sub>1<i>i</i></sub>	$X_{2i}$	$X_{1i} X_{2i}$	$X_{1i}^2$	$X_{2i}^2$
1	1	1	3	3	1	9
2	4	8	5	40	64	25
3	1	3	2	6	9	4
4	3	5	6	30	25	36
;	**	;	;	;	:	-:

Multiply  $X_1$  by  $X_2$  to get  $X_1X_2$ ; then  $X_1^2$ ,  $X_2^2$ . Run regression with Y,  $X_1$ ,  $X_2$ ,  $X_1X_2$ ,  $X_1^2$ ,  $X_2^2$ .

#### R code - multiple linear regression

ibis = read.csv('D:/database/ibisdata/ibis2010.csv', header=T)
head(ibis)

ibis.pre = ibis[ibis\$use==1,c(3:6,8,9,11,12)] head(ibis.pre)

	latitude	aspect	elevation	footprint	year	GDP	рор	slope
1	33.1	0.893	476	61	2008	333	2032	0.503
42	33.3	0.798	484	38	2007	420	3049	0.685
86	33.1	0.56	473	60	2008	256	1485	0.812
104	33.4	0.502	942	20	2006	186	488	5.002
105	33.4	0.502	942	20	2008	186	488	5.002
116	33.2	0.201	476	44	2006	169	1321	2.275

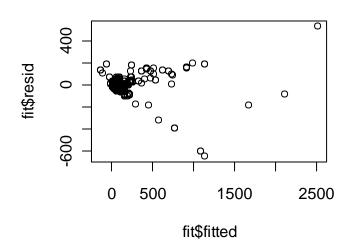
# Multiple Linear Regression Example (only include linear terms)
fit <- Im(pop ~ latitude+elevation+footprint+year+GDP+slope, data=ibis.pre)
summary(fit) # show results

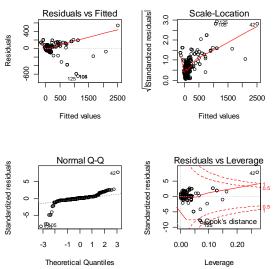
Coefficients:	Estimate	Std.Error	t value	Pr(> t )
(Intercept)	-8670.00000	2120.00000	-4.10000	0.00005
latitude	208.00000	49.80000	4.17000	0.00004
elevation	-0.14400	0.01930	-7.47000	0.00000
footprint	4.43000	0.62400	7.10000	0.00000
year	0.90300	0.64300	1.40000	0.16000
GDP	5.63000	0.11200	50.39000	<0.00000
slope	0.65700	0.54100	1.21000	0.23000

#### R code - multiple linear regression

# Other useful functions
coefficients(fit) # model coefficients
confint(fit, level=0.95) # Cls for model parameters
fitted(fit) # predicted values
residuals(fit) # residuals
anova(fit) # anova table
vcov(fit) # covariance matrix for model parameters

# diagnostic plots
plot(fit\$fitted, fit\$resid)
layout(matrix(c(1,2,3,4),2,2)) # optional 4 graphs
plot(fit)





- GDP

1 16068807 19380852 5596

#### R code - multiple linear regression

```
# Stepwise Regression
> step <- stepAIC(fit, direction="both")
Start: AIC=4658
                                                library(MASS)
pop ~ y + elevation + footprint + year + GDP + slope
                                                fit <- Im(pop ~ y+elevation+footprint+year+GDP+slope,
                                                     data=ibis.pre)
          Df Sum of Sq
                          RSS AIC
         1 9244 3300402 4658
- slope
                                                step <- stepAIC(fit, direction="both")</pre>
- year 1 12344 3303502 4658
                                                step$anova # display results
<none>
                      3291158 4658
    1 108873 3400031 4674
- v
- footprint 1 316173 3607331 4705
                                                # use mtcars data
- elevation 1 349906 3641064 4710
                                               fit <- Im(mpg ~ ., data=mtcars)
- GDP
           1 15920259 19211417 5595
Step: AIC=4658
pop ~ y + elevation + footprint + year + GDP
                                                > step$anova # display results
                                                Stepwise Model Path
          Df Sum of Sq
                          RSS AIC
                                                Analysis of Deviance Table
                11643 3312045 4658
- year
<none>
                      3300402 4658
                                                Initial Model:
+ slope 1 9244 3291158 4658
                                                pop ~ y + elevation + footprint + year + GDP + slope
     1 114255 3414656 4674
- y
- footprint 1 306991 3607392 4703
- elevation 1 346676 3647078 4709
                                                Final Model:
- GDP
      1 15955393 19255794 5594
                                                pop ~ y + elevation + footprint + GDP
Step: AIC=4658
pop ~ y + elevation + footprint + GDP
                                                     Step Df Deviance Resid. Df Resid. Dev AIC
          Df Sum of Sq
                          RSS AIC
                                                                             525
                                                                                    3291158 4658
                      3312045 4658
                                                                            526
<none>
                                                  - slope 1
                                                                 9244
                                                                                    3300402 4658
+ year 1 11643 3300402 4658
                                                                             527
                                                  - year 1
                                                                11643
                                                                                    3312045 4658
+ slope 1 8543 3303502 4658
          1 112618 3424663 4674
- footprint 1 315040 3627084 4704
- elevation 1
               373870 3685915 4713
```

#### Use the full model as a start

M Y0

Y1

#### library(plspm)

#### Path analysis

D = read.csv('d:/data.csv', header=T);D
# path matrix (inner model realtionships)
Y0 = c(0, 0, 0, 0)
Y1 = c(1, 0, 0, 0)
Electro = $c(1, 1, 0, 0)$
SR = c(0,1,1,0)
saker_path = rbind(Y0, Y1, Electro, SR)
# add optional column names

colnames(saker\_path) = rownames(saker\_path)

# plot the path matrix

innerplot(saker\_path)

# list indicating what variables are associated with what latent variables

saker\_blocks = list(c(1,2), c(3,4),c(1,2,3,4),c(5,6))

# all latent variables are measured in a reflective way

 $saker\_modes = rep("A", 4)$ 

# run plspm analysis

saker\_pls = plspm(D, saker\_path, saker\_blocks, modes = saker\_modes)

# what's in saker pls?

saker\_pls

# path coefficients

saker pls\$path coefs

# inner model

saker\_pls\$inner model

# summarized results

summary(saker\_pls)

# plot the results (inner model)

plot(saker pls)

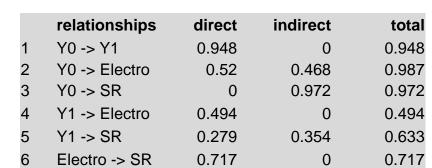
# plot the loadings of the outer model

plot(saker\_pls, what = "loadings", arr.width = 0.2)

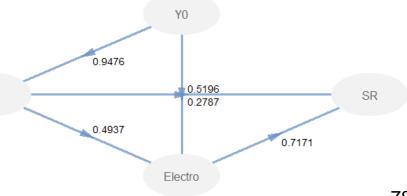
# plot the weights of the outer model

plot(saker pls, what = "weights", arr.width = 0.1)

M_Y0	F_Y0	M_Y1	F_Y1	M_Y2	F_Y2
100	100	80	60	70	50
60	55	40	35	30	30
30	35	15	20	10	12
62	60	50	40	38	35
40	45	30	35	25	27
70	65	60	35	50	30
50	45	45	40	32	28
55	60	42	45	31	32



number of males at Year 0



# Multiple correlation

# Multiple correlation coefficient

- Correlation coefficient in the context of multiple regression
- R can be defined as the correlation between the criterion (Y) and the best linear combination of the predictors

$$R = r_{Y\hat{Y}}$$

$$\hat{Y} = b_0 + b_1 X_1 + b_2 X_2 + \dots + b_p X_p$$

## Partitioning of variance

 Sum of squares that is related to regression (SSR):

$$\sum (\hat{Y}_i - \overline{Y})^2 = SS_{\hat{Y}}$$

• Sum of squares that is related to **residual** (error; SSE):  $\sum_{i} (Y_i - \hat{Y}_i)^2 = SS_{\text{residual}}$ 

• Sum of squares related to *total* deviation (SST):

$$\sum (Y_i - \overline{Y})^2 = SS_Y$$

## Multiple correlation coefficient (squared)

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

- R<sup>2</sup> can be interpreted in terms of percentage of accountable variation
- R<sup>2</sup> = 0.755: we can say that 75.5% of the variation in Y can be predicted on the basis of the Xs

## Partial regression coefficients

Coefficients in multiple regression are called partial regression coefficients

$$\hat{Y} = b_0 + b_1 X_1 + b_2 X_2 + \dots + b_p X_p$$

- Example:  $b_1$  is coefficient for regression of Y on  $X_1$  when we **partial out** the effect of  $X_2, ..., X_p$ 
  - When other variables are held constant
- Common mistake: equate b<sub>1</sub> in the context of the other X<sub>i</sub> with the simple regression coefficient when ignoring X<sub>i</sub>.

## **Partial correlation**

Partial correlation measures the degree of association between two random variables, with the effect of a set of controlling random variables (e.g.,  $x_2$ ) removed for both variables (e.g., y and y)

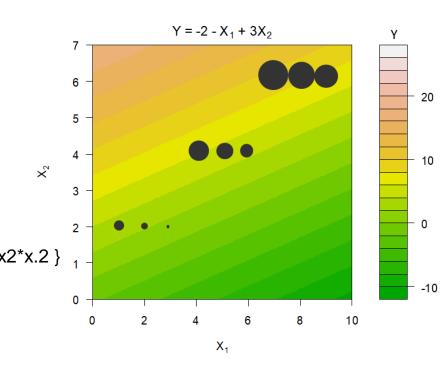
$$y = X_1 + X_2$$

$$Partial_{y} = \frac{r_{y1} - (r_{y2})(r_{12})}{\sqrt{1 - r_{y2}^2} \sqrt{1 - (r_{12})^2}}$$

Semi - Partial<sub>y1</sub> = 
$$\frac{r_{y1} - (r_{y2})(r_{12})}{\sqrt{1 - (r_{12})^2}}$$

# Partial correlation example

```
y < -c(3, 2, 1, 6, 5, 4, 9, 8, 7)
x1 \leftarrow c(1, 2, 3, 4, 5, 6, 7, 8, 9)
x2 \leftarrow c(2, 2, 2, 4, 4, 4, 6, 6, 6)
# multiple regression
fit = summary(Im(y \sim x1 + x2))
interception = fit[[4]][1,1]
coef x1
              = fit[[4]][2,1]
coef x2
              = fit[[4]][3,1]
x.1 <- seq(min(x1) -1, max(x1) + 1, length = 100)
x.2 <- seq(min(x2) -2, max(x2) + 1, length = 100)
f \leftarrow function(x.1, x.2) \{ r \leftarrow interception + coef_x1*x.1 + coef_x2*x.2 \}
y.pred \leftarrow outer(x.1, x.2, f)
filled.contour(x.1, x.2, y.pred, main="", color = terrain.colors,
              xlab=expression(paste(X[1])),
              ylab=expression(paste(X[2])),
              ylim=c(1, 7)
points(x1/1.3, x2, pch=16, cex=y)
library(ggm)# partial correlation
D = cbind(y, x1, x2)
D = jitter(D, factor = .01)
pcor(c("y", "x1"), var(D)) # 0.8
pcor(c("y", "x1", "x2"), var(D)) # -0.9999
```



## R code - partial correlation

```
# partial correlation
library(ggm)
## The marginal correlation between analysis and statistics
pcor(c("footprint", "GDP"), var(ibis.pre))
cor(ibis.pre$footprint, ibis.pre$GDP)
0.528
## The correlation between footprint and GDP given elevation
pcor(c("footprint", "GDP", "elevation"), var(ibis.pre))
0.507
## The correlation between footprint and GDP given elevation and latitude
pcor(c("footprint", "GDP", "elevation", "latitude"), var(ibis.pre))
0.5
```

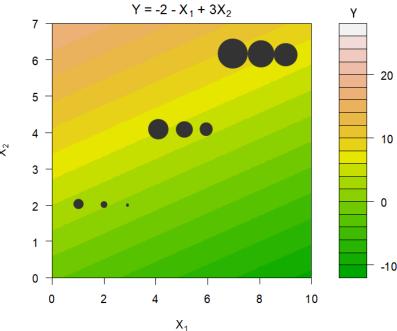
# Partial correlation example

• For any *fixed* value of  $X_2$ , slope of the regression line of Y on  $X_1$  is negative (in fact  $b_{01.2} = -0.99$ )

• However, regression of Y on  $X_1$  when **ignoring**  $X_2$  is

positive ( $b_{01} = 0.8$ )

Partialling out and ignoring are very different!



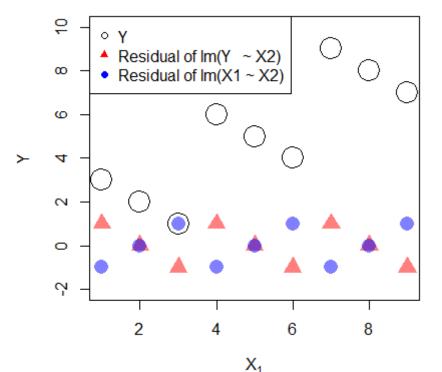
When X<sub>1</sub> and X<sub>2</sub> are independent,
 regression coefficients will be equal in both cases

# Remove the effect of X<sub>2</sub>

- Suppose we regress Y on  $X_2$  and obtain the residual values  $Y_r = Y_i \hat{Y}_i$
- Residual values represent part of Y that cannot be predicted by X<sub>2</sub>: *independent* of X<sub>2</sub>
- Now regress  $X_1$  on  $X_2$  generating  $X_{1r} = X_{1i} \hat{X}_{1i}$
- Again, residual values represent part of X<sub>1</sub> that is independent of X<sub>2</sub>
- We now have two sets of residuals: part of Y and part of X<sub>1</sub> that are *independent* of X<sub>2</sub>
  - Partialled  $X_2$  out of Y and out of  $X_1$

# Remove the effect of X<sub>2</sub>

- Now regress Y<sub>r</sub> on X<sub>1r</sub>: regression coefficient will be the partial coefficient b
- Correlation between  $Y_r$  and  $X_{1r}$  is the **partial correlation** of Y and  $X_1$ , with  $X_2$  partialled out:  $r_{01,2}$



$$b_{Y_r X_{1r}} = \frac{\text{cov}_{Y_r X_{1r}}}{s_{X_1}^2} = -1$$

# Contribution, fraction, partial R<sup>2</sup>

- Contribution of a variable x<sub>j</sub> to the explanation of the variation of a dependent variable y.
- Fraction [a] in variation partitioning.
- Partial  $R^2$  (partial determination coefficient) between an  $x_j$  and a y variable.

### Contribution

Scherrer (1984) called the quantity  $a_j * r_{yxj}$  the "contribution" of the *j*-th variable to the explanation of the variance of y;

- $-a_{j}$  is the standardized regression coefficient of the j-th explanatory variable,
- $-r_{yxj}$  is the simple correlation coefficient (Pearson r) between y and  $x_i$ .

# Fraction [a] in variation partitioning

### semipartial correlation squared

- This fraction measures the proportion of the variance of y explained by the explanatory variable  $x_1$  (for example) when the other explanatory variables ( $x_2$ ,  $x_3$ ...) are held constant with respect to  $x_1$  only (and not with respect to y).
- Thus, one obtains fraction [a] by examining the r<sup>2</sup>
   obtained by regressing y on the residuals of a regression
   of x<sub>1</sub> on x<sub>2</sub>, x<sub>3</sub>...

### Partial R<sup>2</sup>

- The partial R measures the mutual relationship between two variables y and x<sub>j</sub> when other variables (x<sub>1</sub>, x<sub>2</sub>, x<sub>3</sub>...) are held constant with respect to the two variables involved y and x<sub>j</sub>
- The **partial**  $R^2$  is the square of the partial R above. For  $y = x_1 + x_2$ , it measures the proportion of the variance of the residuals of y with respect to  $x_2$  that is explained by the residuals of  $x_1$  with respect to  $x_2$ .

#### R code for contribution, fraction, partial R<sup>2</sup> and variance partitioning

```
mtcars; mtcars.st = scale(mtcars); apply(mtcars.st, 2, var)
mtcars.st = as.data.frame(mtcars.st)
fit = Im(mpg \sim cyl + disp + hp + drat + wt + qsec + vs + am + gear + carb, data=mtcars.st)
# Contribution
Contribution = coef(fit) * cor(mtcars.st)[1,]
fit2 = step(fit)
Contribution = coef(fit2)[-1] * cor(mtcars.st)[1, c(6,7,9)]
# Fraction
f.wt = Im(wt \sim qsec + am, data=mtcars.st)
res.wt = resid(f.wt)
Fraction.a = summary(lm(mtcars.st$mpg ~ res.wt))$r.squared
# Partial.R2
f.mpg = Im(mpg ~ qsec + am, data=mtcars.st)
res.mpg = resid(f.mpg)
Partial.R2 = summary(lm(res.mpg ~ res.wt))$r.squared
# Variance partition
fit = Im(mpg ~ wt + qsec + am, data=mtcars.st)
anova(fit)[[2]] / sum(anova(fit)[[2]])
```

	wt	qsec	am
Contribution	0.5516	0.1521	0.1458
Fraction [a]	0.1628	0.0968	
Partial R <sup>2</sup>	0.5199	0.1175	
Variance	0.7528	0.0735	0.0232

'wt' (car weight measured in tons) 'gsec' (the number of second a car takes to reach .25 miles) 'am' (transmission type)

### Canonical correlation analysis

- In CCA, there can be multiple response variables.
- Canonical correlations are the maximum correlation between a linear combination of the responses and a linear combination of the predictor variables.

Given a linear combination of X variables:

$$F = f_1 X_1 + f_2 X_2 + ... + f_p X_p$$

and a linear combination of Y variables:

$$G = g_1 Y_1 + g_2 Y_2 + ... + g_q Y_q$$

The first canonical correlation is:

Maximum correlation coefficient between *F* and *G*, for all *F* and *G* 

$$F_1 = \{f_{11}, f_{12}, \dots, f_{1p}\}$$
 and  $G_1 = \{g_{11}, g_{12}, \dots, g_{1q}\}$  are corresponding **canonical variates**

#### One example of CCA

# http://www.ats.ucla.edu/stat/r/dae/canonical.htm

```
require(ggplot2)
require(GGally)
require(CCA)
```

# Example 1. A researcher has collected data on three psychological variables, four academic variables (standardized test scores) # and gender for 600 college freshman. She is interested in how the set of psychological variables relates to the academic # variables and gender. In particular, the researcher is interested in how many dimensions (canonical variables) are necessary to # understand the association between the two sets of variables.

```
mm <- read.csv("http://www.ats.ucla.edu/stat/data/mmreg.csv")
colnames(mm) <- c("Control", "Concept", "Motivation", "Read", "Write", "Math", "Science", "Sex")
summary(mm); head(mm)
```

psych <- mm[, 1:3] acad <- mm[, 4:8]	
ggpairs(psych) ggpairs(acad)	

Control	Concept	Motivation	Read	Write	Math	Science	Sex
-0.84	-0.24	1	54.8	64.5	44.5	52.6	1
-0.38	-0.47	0.67	62.7	43.7	44.7	52.6	1
0.89	0.59	0.67	60.6	56.7	70.5	58	0
0.71	0.28	0.67	62.7	56.7	54.7	58	0
-0.64	0.03	1	41.6	46.3	38.4	36.3	1
1.11	0.9	0.33	62.7	64.5	61.4	58	1

# correlations within and between the two sets of variables matcor(psych, acad) #CCA package

## Sex

-0.3641

#### One example of CCA

```
# Canonical Correlation Analysis
cc1 <- cc(psych, acad)
summary(cc1)
##
             Length
                          Class
                                       Mode
## cor
                                       numeric
                          -none-
## names
                                       list
                          -none-
## xcoef
                                       numeric
                          -none-
## ycoef
             15
                          -none-
                                       numeric
## scores
                                       list
                          -none-
# display the canonical correlations
cc1$cor
## [1] 0.4641
               0.1675
                        0.1040
# raw canonical coefficients
cc1[3:4]
## $xcoef
##
                  [,1]
                            [,2]
                                         [,3]
               -1.2538
                          -0.6215
## Control
                                       -0.6617
## Concept
               0.3513
                          -1.1877
                                       0.8267
## Motivation
               -1.2624
                          2.0273
                                       2.0002
##
## $ycoef
##
                  [,1]
                             [,2]
                                         [,3]
                          -0.004910
                                      0.021381
## Read
              -0.044621
              -0.035877
                          0.042071
## Write
                                      0.091307
## Math
               -0.023417 0.004229
                                      0.009398
## Science
              -0.005025 -0.085162
                                     -0.109835
## Sex
               -0.632119 1.084642 -1.794647
```

```
# compute canonical loadings
cc2 <- comput(psych, acad, cc1)
# display canonical loadings
cc2[3:6]
## $corr.X.xscores
##
                 [,1]
                          [,2]
                                  [,3]
## Control
                       -0.3897 -0.1756
              -0.90405
## Concept
             -0.02084 -0.7087 0.7052
## Motivation -0.56715
                        0.3509 0.7451
##
## $corr.Y.xscores
##
                 [,1]
                          [,2]
                                    [,3]
## Read
              -0.3900
                       -0.06011
                                  0.01408
## Write
              -0.4068
                       0.01086
                                 0.02647
## Math
              -0.3545
                       -0.04991
                                 0.01537
## Science
              -0.3056
                       -0.11337 -0.02395
## Sex
               -0.1690
                        0.12646 -0.05651
##
## $corr.X.yscores
##
                                     [,3]
                 [,1]
                          [,2]
## Control
              -0.419555 -0.06528
                                  -0.01826
## Concept
             -0.009673 -0.11872
                                  0.07333
## Motivation -0.263207 0.05878
                                  0.07749
##
## $corr.Y.yscores
##
                                [,3]
             [,1]
                       [,2]
           -0.8404
                              0.1354
## Read
                    -0.35883
## Write
           -0.8765
                    0.06484 0.2546
## Math
           -0.7639
                    -0.29795 0.1478
## Science
           -0.6584
                    -0.67680 -0.2304
```

#### One example of CCA

In general, the number of canonical dimensions is equal to the number of variables in the smaller set, however, the number of significant dimensions may be even smaller.

Canonical dimensions, also known as canonical variates, are latent variables that are analogous to factors obtained in factor analysis.

For this particular model there are three canonical dimensions of which only the first two are statistically significant.

```
# tests of canonical dimensions
ev <- (1 - cc1$cor^2)
n <- dim(psych)[1]
p <- length(psych)
q <- length(acad)
k \leftarrow min(p, q)
m < -n - 3/2 - (p + q)/2
w <- rev(cumprod(rev(ev)))
# initialize
d1 <- d2 <- f <- vector("numeric", k)
for (i in 1:k) {
 s \leftarrow sqrt((p^2 * q^2 - 4)/(p^2 + q^2 - 5))
 si <- 1/s
 d1[i] <- p * q
 d2[i] <- m * s - p * q/2 + 1
 r <- (1 - w[i]^si)/w[i]^si
 f[i] <- r * d2[i]/d1[i]
 p < -p - 1
 q < -q - 1
pv \leftarrow pf(f, d1, d2, lower.tail = FALSE)
(dmat \leftarrow cbind(WilksL = w, F = f, df1 = d1, df2 = d2, p = pv))
```

## **Assignment**

General objectives: learn about multiple linear regression.

- Develop a dataset to perform:
  - Multiple linear regression

Y-X1, X2, X3, etc.

- Check R<sup>2</sup>, significance of each variables, multicollinearity, homogeneous of residuals
- Briefly interpret the results

#### R code – correlation plot

## put (absolute) correlations on the upper panels,

