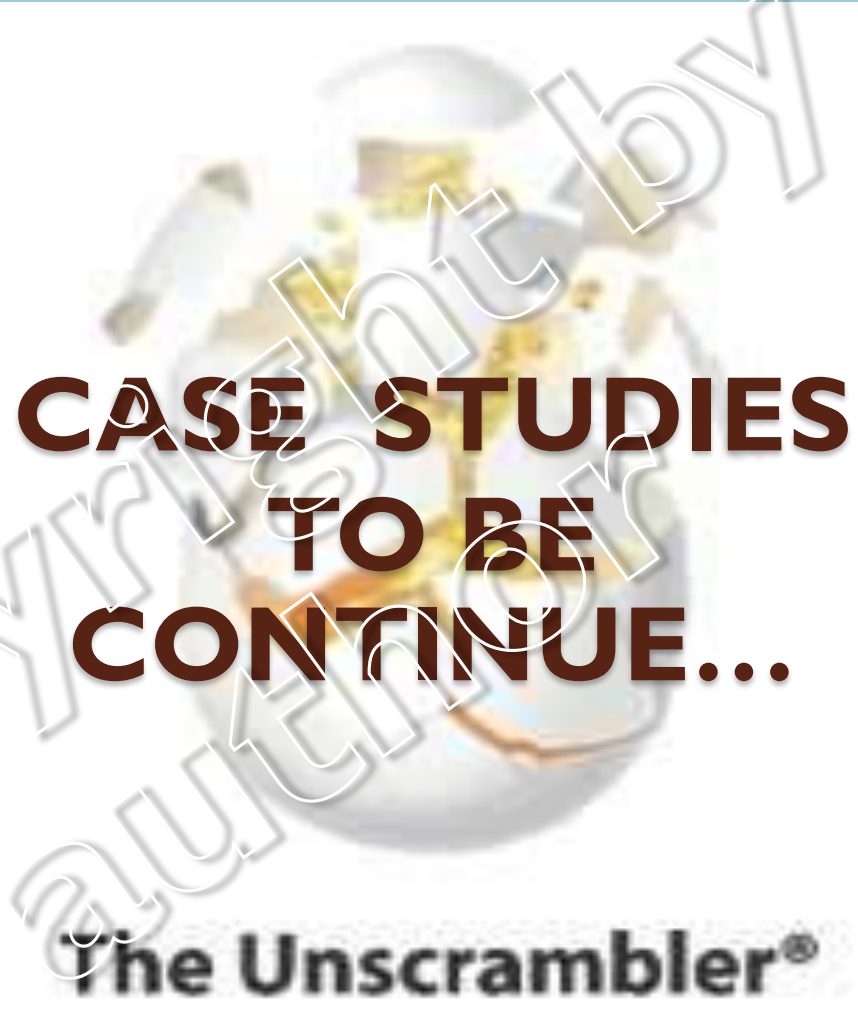


• สื่อการสอนเรื่อง “**Chemometrics**” นี้
จัดทำขึ้นโดย ดร.ศุมาพร เกษมสำราญ
สำหรับประกอบการสัมมนา

หัวข้อ “การใช้ **Unscrambler** วิเคราะห์
ข้อมูลเพื่อหาค่าองค์ประกอบของผลิตภัณฑ์”
จัดโดยบริษัท จาร์พา เทคโนโลยีเตอร์ จำกัด
วันพฤหัสบดี ที่ 11 กันยายน 2551
มหาวิทยาลัยเกษตรศาสตร์



**CASE STUDIES
TO BE
CONTINUE...**

The Unscrambler®

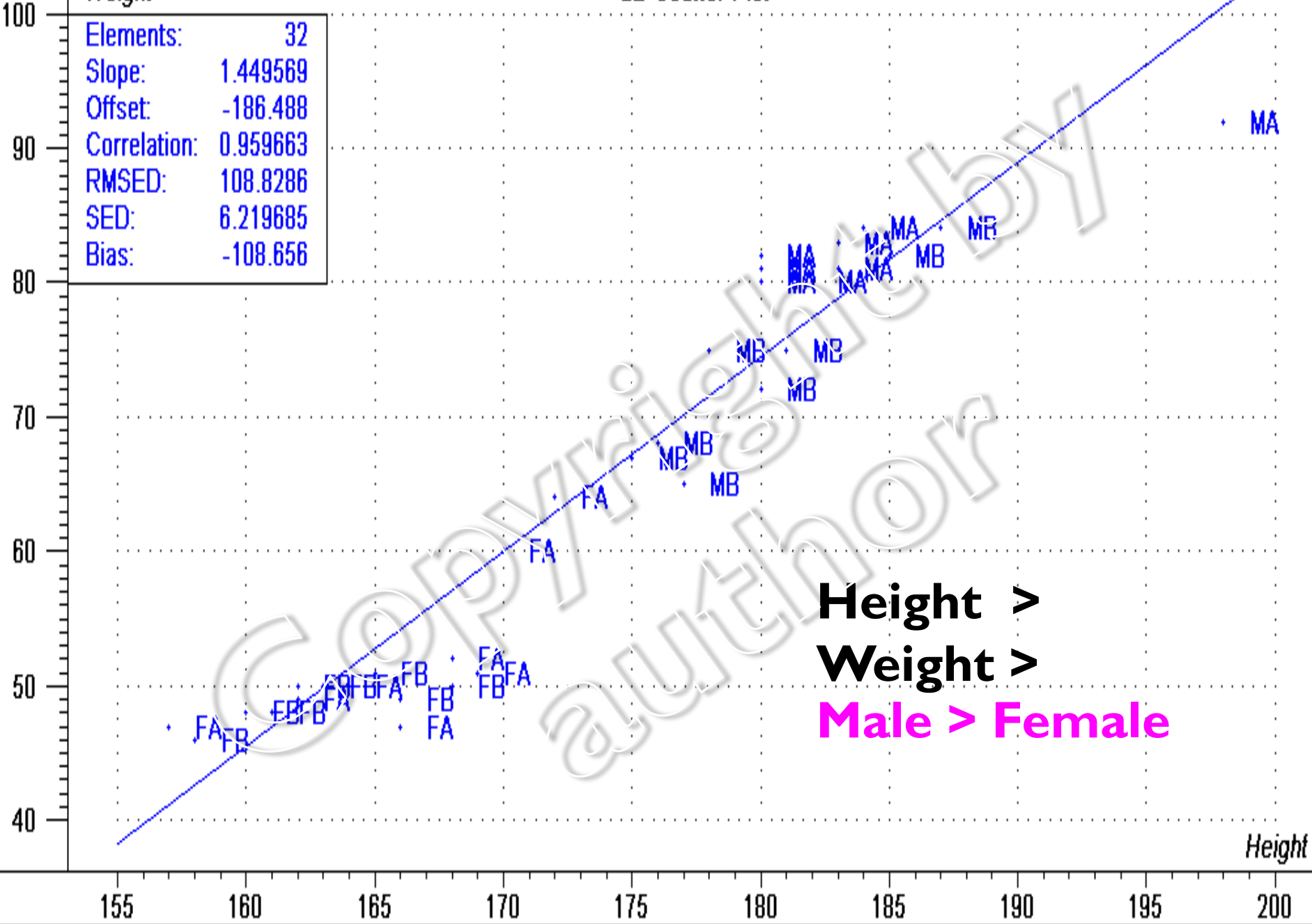
Case I. Relationship of variables

- “PEOPLE” - data
- (Multivariate Data Analysis-in practice, CAMO)

Height	cm.
Weight	kg.
Hair length	Short = -1, long = +1
Shoe size	EU standard
Age	Years
Income	Euro
Beer consumption	Liters per year
Wine consumption	Liters per year
Sex	Male = -1, female = +1
Swimming ability	500 m timed swimming
Regional belonging	A=-1=Scandinavia, B=+1=Mediterranean
IQ	EU standard

2D Scatter Plot

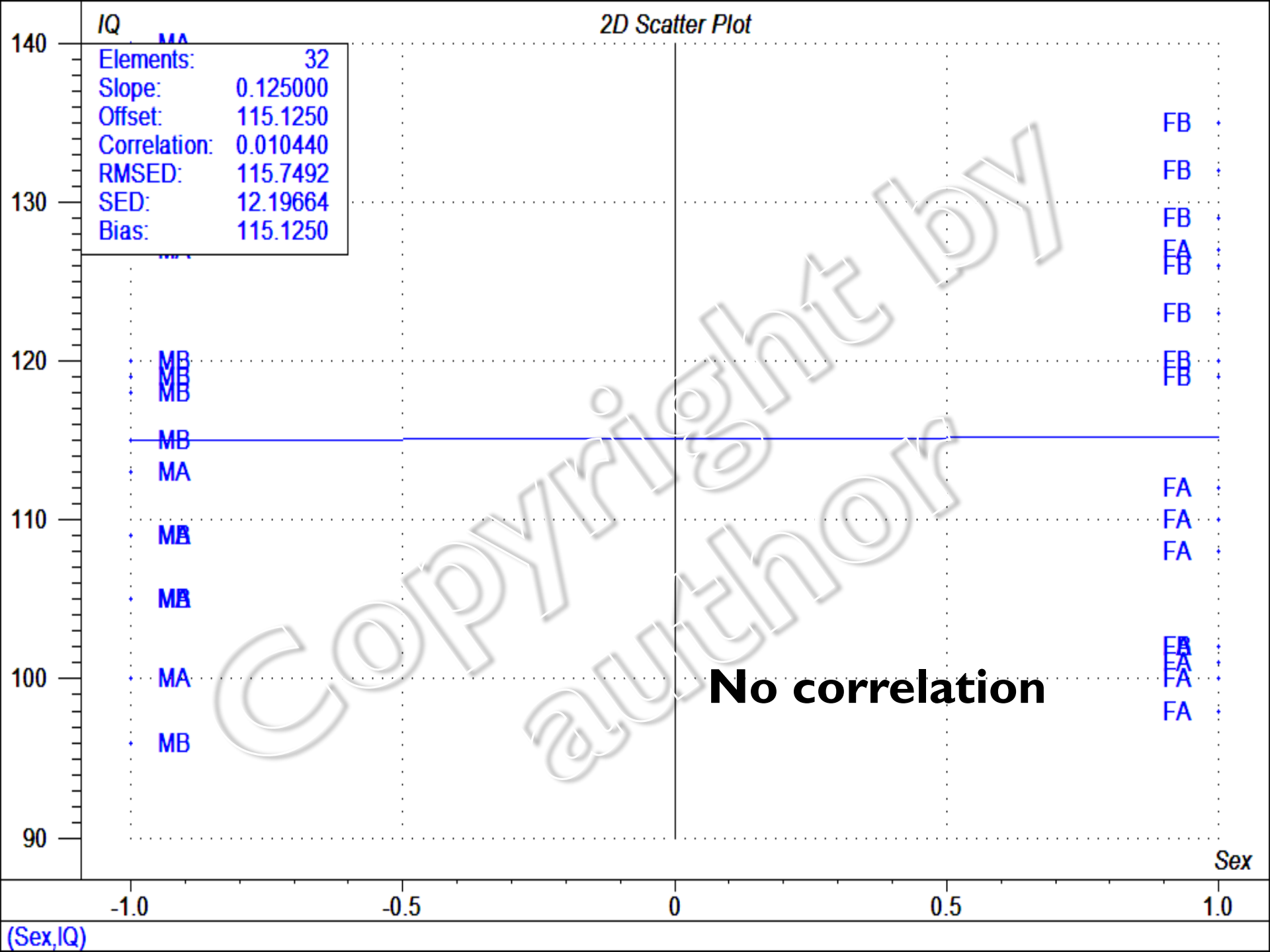
Weight	
Elements:	32
Slope:	1.449569
Offset:	-186.488
Correlation:	0.959663
RMSED:	108.8286
SED:	6.219685
Bias:	-108.656



(Height,Weight)

2D Scatter Plot

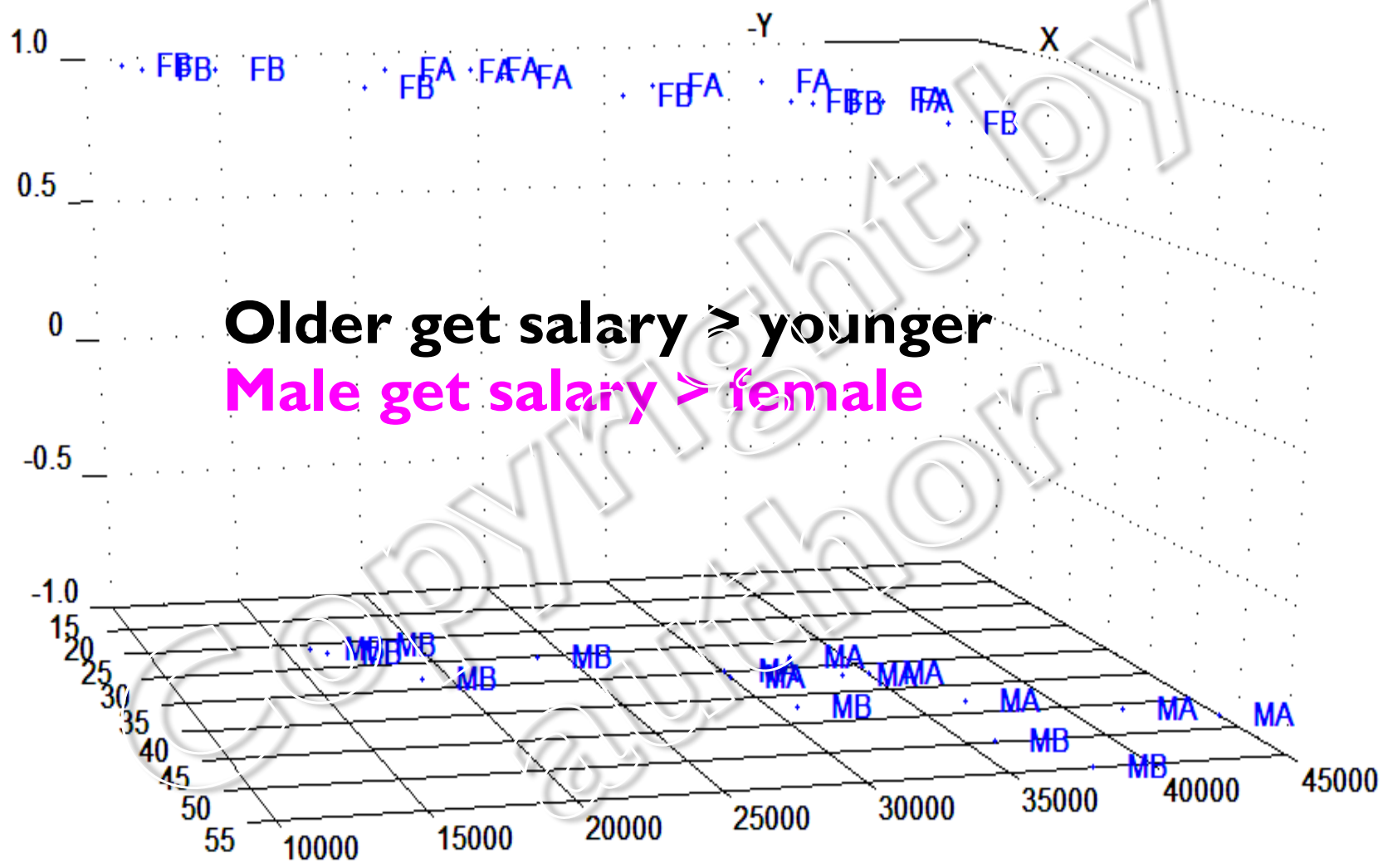
IQ
Elements: 32
Slope: 0.125000
Offset: 115.1250
Correlation: 0.010440
RMSED: 115.7492
SED: 12.19664
Bias: 115.1250



No correlation

(Sex,IQ)

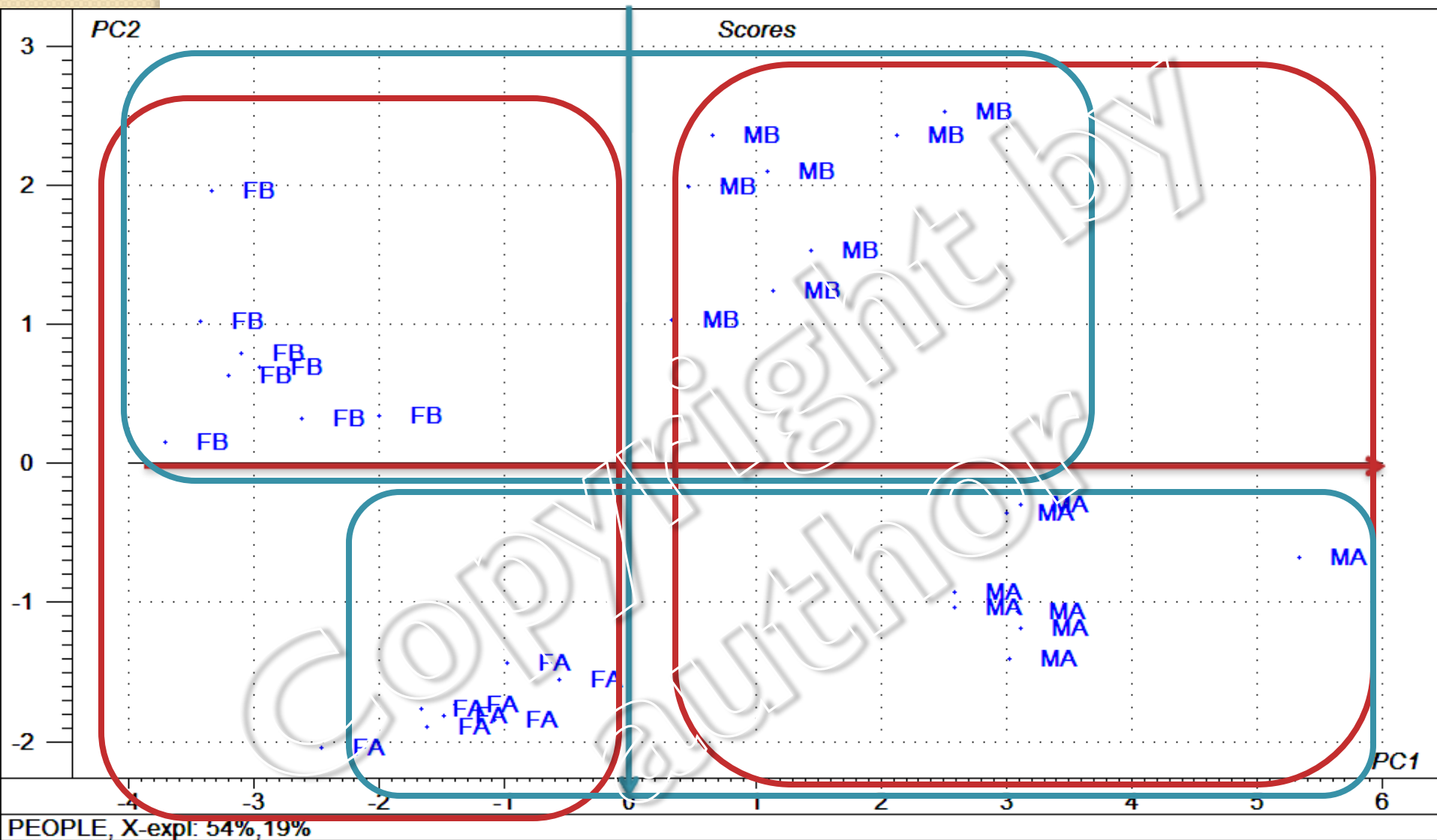
3D Scatter Plot



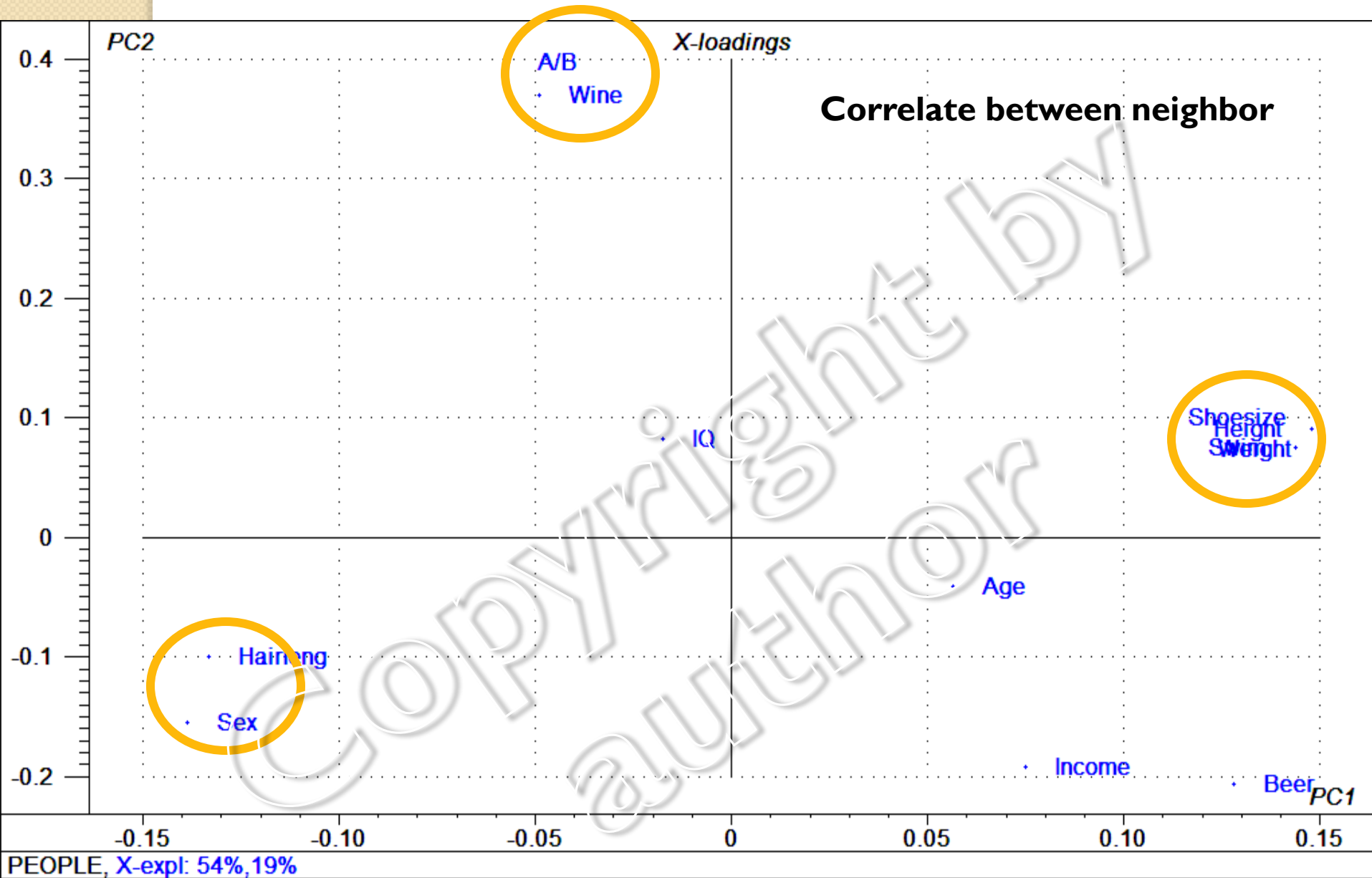
X, Y, Z

(Age, Income, Sex)

PC I : Sex discrimination

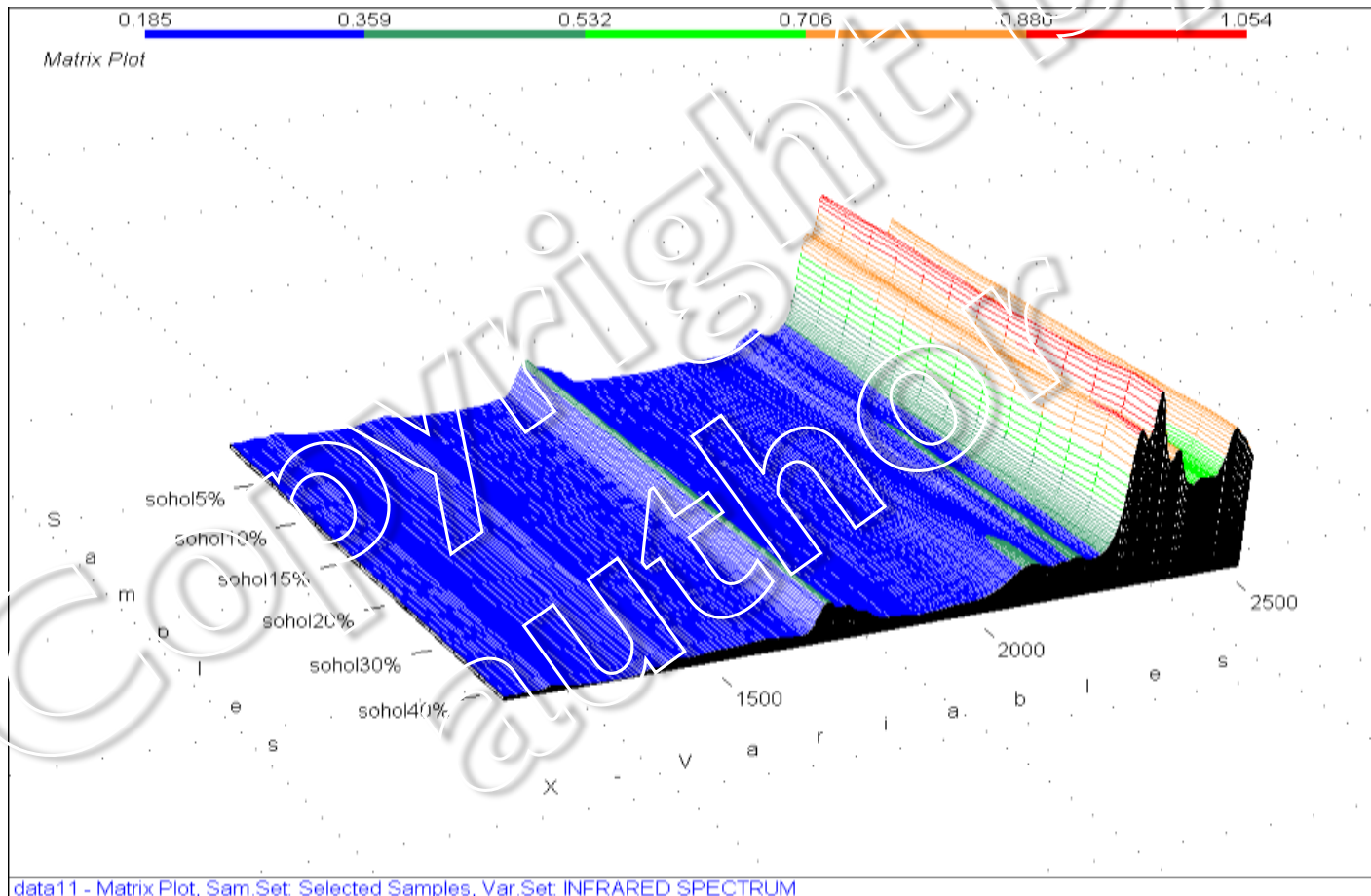


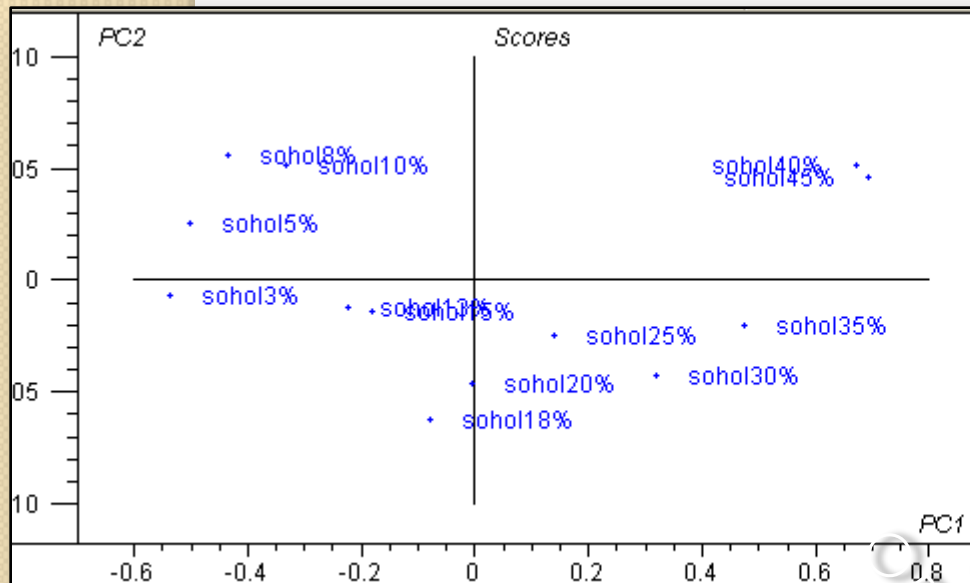
PC 2 : Region discrimination



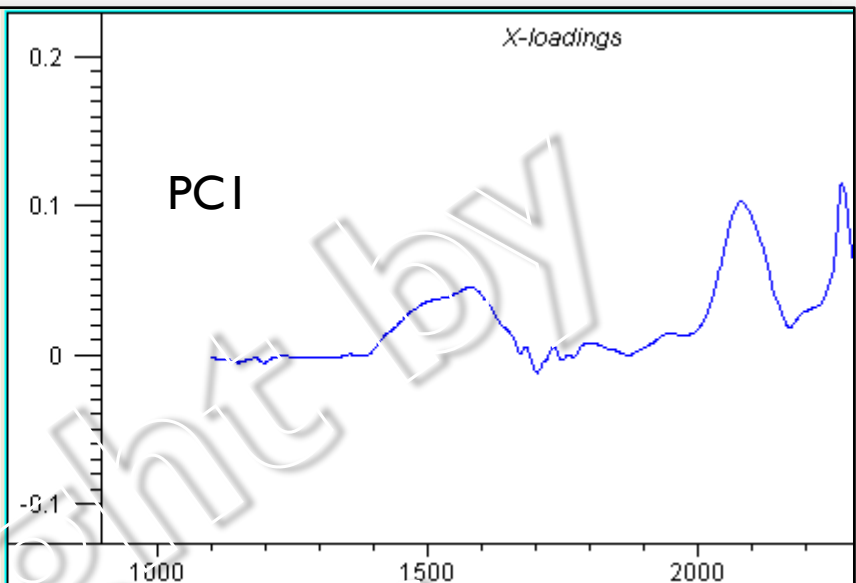
Case 2. PLS

- “Gasohol” – data
- Matrix size of 13 x 701

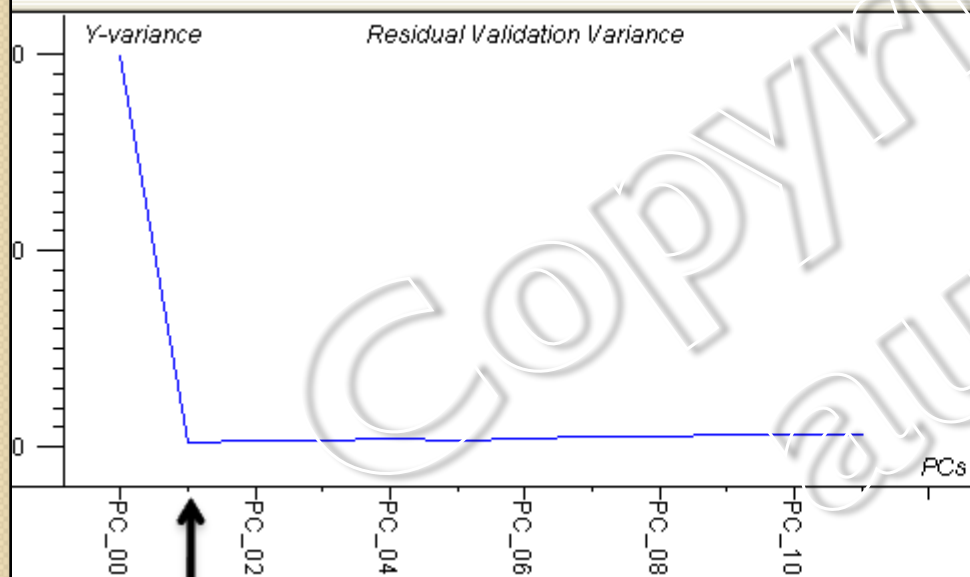




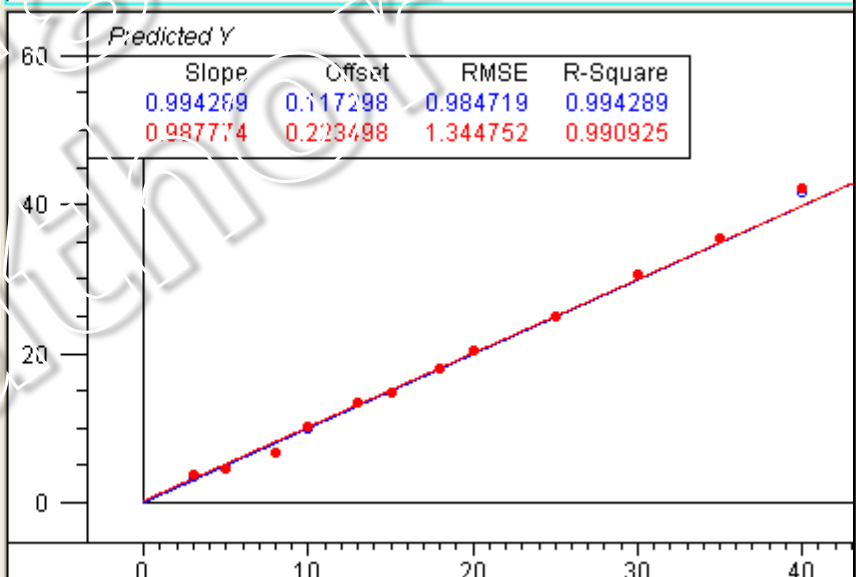
SULT1, X-expl: 99%,1% Y-expl: 99%,0%



RESULT1, PC(X-expl,Y-expl): 1(99%,99%)



SULT1, Variable: v.Total



RESULT1, (Y-var, PC): (ethanol,1) (ethanol,1)

Ethanol absorption bands

First overtone band

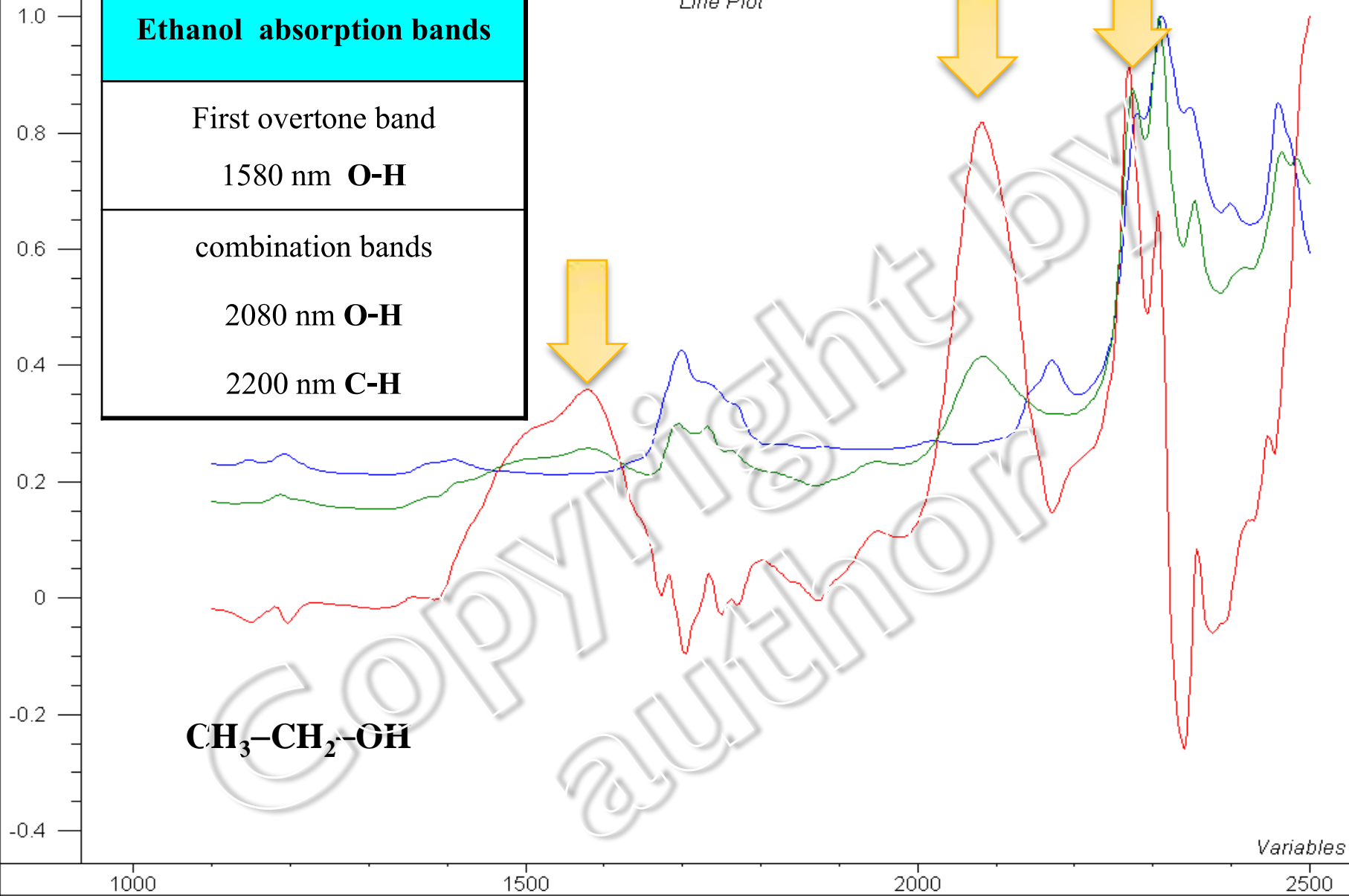
1580 nm O-H

combination bands

2080 nm O-H

2200 nm C-H

Line Plot



benz95 (X-Variables) PC_01 (X-Variables) ethanol100% (X-Variables)

Case 3. Classification

“IRIS” - data

(Multivariate Data Analysis-in practice, CAMO)

Matrix size of 150 x 4

3 Groups



Iris Setosa

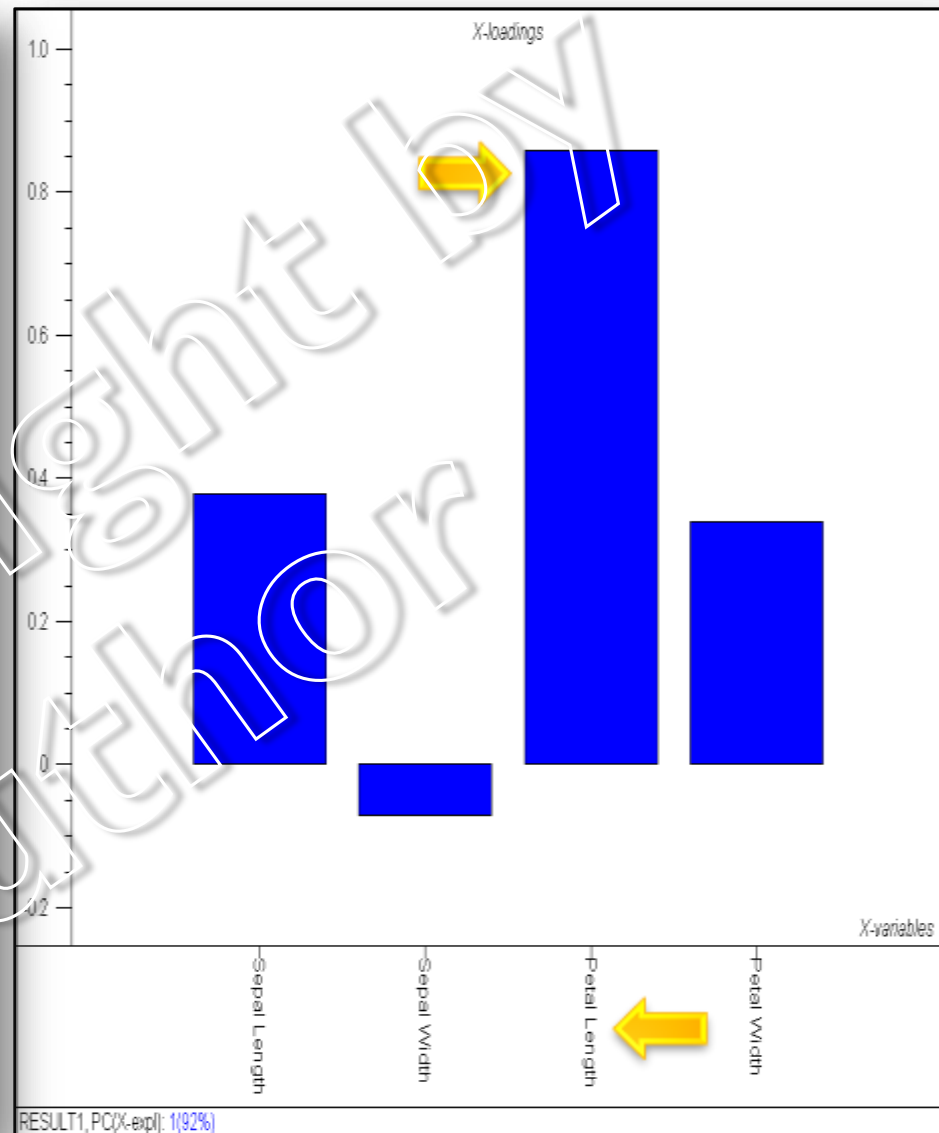
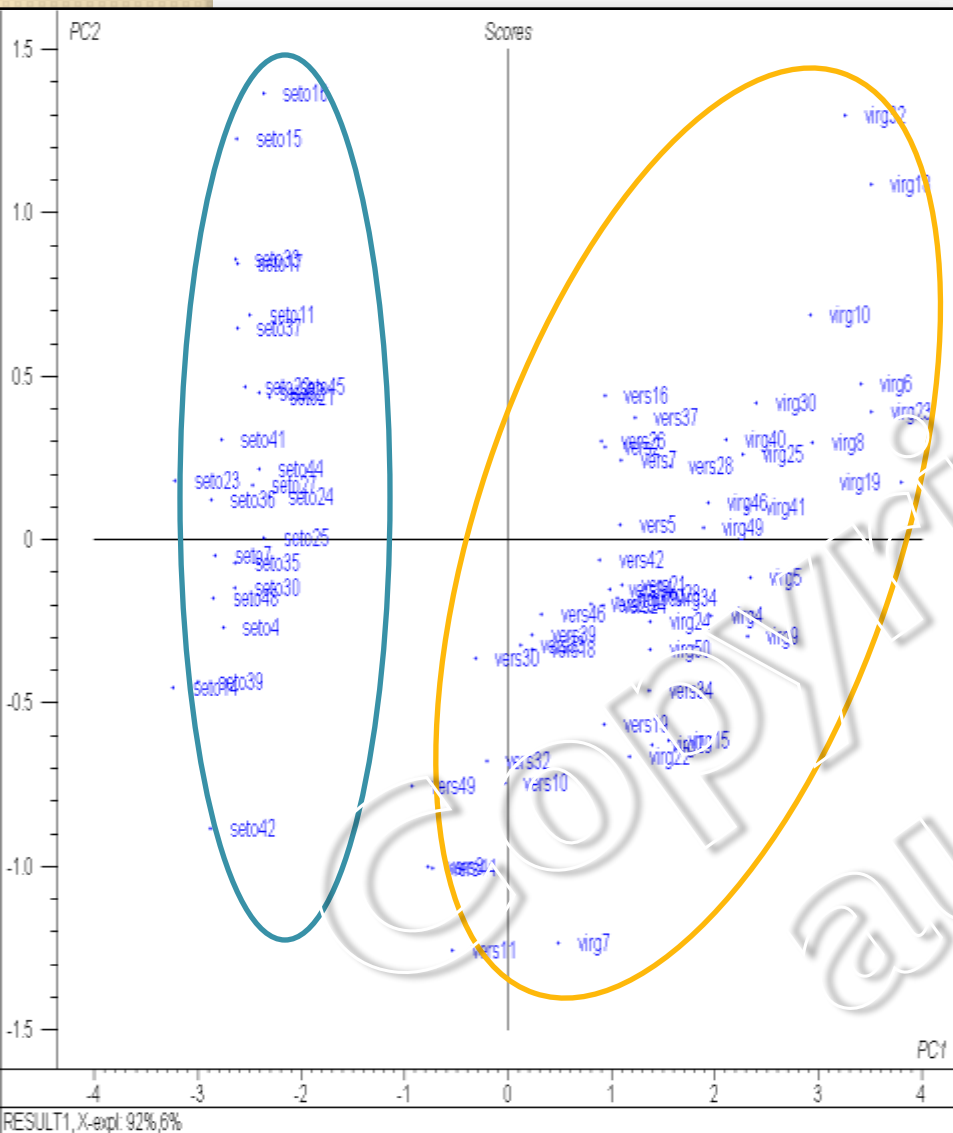


Iris Virginica



Iris Versicolor

3.1 PCA



• 3.2 SIMCA

		Sepal Length	Sepal Width	Petal Length	Petal Width	Type
		1	2	3	4	5
seto29	118	5.2000	3.4000	1.4000	0.2000	Setosa
seto31	119	4.8000	3.1000	1.6000	0.2000	Setosa
seto34	120	5.5000	4.2000	1.4000	0.2000	Setosa
seto38	121	4.9000	3.6000	1.4000	0.2000	Setosa
seto40	122	5.1000	3.4000	1.5000	0.2000	Setosa
seto43	123	4.4000	3.2000	1.3000	0.2000	Setosa
seto46	124	4.8000	3.0000	1.4000	0.2000	Setosa
seto47	125	5.1000	3.8000	1.6000	0.2000	Setosa
virg1	126	6.3000	3.3000	6.0000	2.3000	Virginica
virg3	127	7.1000	3.0000	5.9000	2.4000	Virginica
virg11	128	6.5000	3.2000	5.1000	2.5000	Virginica
virg12	129	6.4000	2.7000	5.3000	2.6000	Virginica
virg13	130	6.8000	3.0000	5.5000	2.7000	Virginica
virg14	131	5.7000	2.5000	5.0000	2.2000	Virginica
virg16	132	6.4000	3.2000	5.3000	2.4000	Virginica
virg17	133	6.5000	2.6000	5.5000	2.5000	Virginica
virg20	134	6.0000	2.2000	5.0000	2.3000	Virginica
virg21	135	6.9000	3.2000	5.7000	2.4000	Virginica
virg26	136	7.2000	3.2000	6.0000	2.5000	Virginica
virg27	137	5.2000	2.8000	4.8000	2.1000	Virginica
virg29	138	6.4000	2.8000	5.6000	2.2000	Virginica
virg31	139	7.4000	2.9000	6.1000	2.3000	Virginica
virg33	140	6.4000	2.8000	5.6000	2.4000	Virginica
virg35	141	6.1000	2.6000	5.8000	2.5000	Virginica
virg36	142	7.7000	3.0000	6.1000	2.6000	Virginica
virg37	143	6.3000	3.4000	5.6000	2.7000	Virginica
virg38	144	6.4000	3.1000	5.5000	2.8000	Virginica
virg42	145	6.9000	3.1000	5.1000	2.3000	Virginica
virg43	146	5.8000	2.4000	5.1000	1.9000	Virginica
virg44	147	6.8000	3.2000	5.9000	2.3000	Virginica
virg45	148	6.7000	3.3000	5.7000	2.5000	Virginica
virg47	149	6.3000	2.5000	5.0000	1.9000	Virginica
virg48	150	6.5000	3.0000	5.2000	2.0000	Virginica

Principal Component Analysis

Samples Variables

Sample Set: Setosa [25] Define...

Keep Out of Calculation: Select...

Frozen Calibration Samples: Select...

Validation Method

Leverage Correction

Cross Validation Setup...

Uncertainty test: ... PCs ...

Test Set Setup...

Model Size: Full Num PCs: 4

Center Data

Add Start Noise

Issue Warnings Warning Limits...

OK Cancel Help

		Sepal Length	Sepal Width	Petal Length	Petal Width	Type
		1	2	3	4	5
seto43	123	4.4000	3.2000	1.3000	0.2000	Setosa
seto46	124	4.8000	3.0000	1.4000	0.3000	Setosa
seto47	125	5.1000	3.8000	1.6000	0.2000	Setosa
virg1	126	6.3000	3.3000	6.0000	0.5000	Virginica
virg3	127	7.1000	3.0000	5.9000	0.5000	Virginica
virg11	128	6.5000	3.2000	5.1000	0.5000	Virginica
virg12	129	6.4000	2.7000	5.3000	0.5000	Virginica
virg13	130	6.8000	3.0000	5.5000	0.5000	Virginica
virg14	131	5.7000	2.5000	5.0000	0.5000	Virginica
virg16	132	6.4000	3.2000	5.3000	0.5000	Virginica
virg17	133	6.5000	3.0000	5.5000	0.5000	Virginica
virg20	134	6.0000	2.2000	5.0000	0.5000	Virginica
virg21	135	6.9000	3.2000	5.7000	0.5000	Virginica
virg26	136	7.2000	3.2000	6.0000	0.5000	Virginica
virg27	137	6.2000	2.8000	4.8000	0.5000	Virginica
virg29	138	6.4000	2.8000	5.5000	0.5000	Virginica
virg31	139	7.4000	2.8000	6.1000	0.5000	Virginica
virg33	140	6.4000	2.8000	5.6000	0.5000	Virginica
virg35	141	6.1000	2.8000	5.6000	0.5000	Virginica
virg36	142	7.7000	3.0000	6.1000	0.5000	Virginica
virg37	143	6.3000	3.4000	5.6000	0.5000	Virginica
virg38	144	6.4000	3.1000	5.5000	0.5000	Virginica
virg42	145	6.9000	3.1000	5.1000	0.5000	Virginica
virg43	146	5.8000	2.4000	5.1000	0.5000	Virginica
virg44	147	6.8000	3.2000	5.9000	0.5000	Virginica
virg45	148	6.7000	3.3000	5.7000	0.5000	Virginica
virg47	149	6.3000	2.5000	5.9000	0.5000	Virginica
virg48	150	6.5000	3.0000	5.2000	2.0000	Virginica

Classification

Samples | X-variables | Pretreat Vars

Sample Set: Training [75] Define...

Keep Out of Calculation: Select...

Centered Models

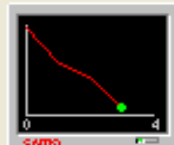
Model	Method	Number of PC's			#Pret
		Max	Sugg	Use	
PCA_Setosa	PCA	4	3	1	0
PCA_Versicolor	PCA	4	3	1	0
PCA_Virginica	PCA	4	3	1	0

Number of PC's to Use: 1

Add Model... Remove Model

OK Cancel Help

Variance... Pretreat...



Classification Table

Sample	PCA_Setosa	PCA_Ver...	PCA_Vir...
seto27	*		
seto30	*		
seto32	*		
seto33	*		
seto35	*		
seto36	*		
seto37	*		
seto39	*		
seto41	*		
seto42	*		
seto45	*		
seto48	*		
seto14	*		
seto16	*		
seto25	*		
seto44	*		
virg2			*
virg4	*	*	
virg5			*
virg6			*
virg7			*
virg8			*
virg9			*
virg10			*
virg15			*
virg18			*
virg19			*
virg22			*
virg23			*
virg24	*	*	
virg25			*
virg28	*	*	
virg30	*	*	
virg32	*	*	
virg34	*	*	
virg39	*	*	
virg40	*	*	

Correct classification

Correct classification

Doubly classified, see also

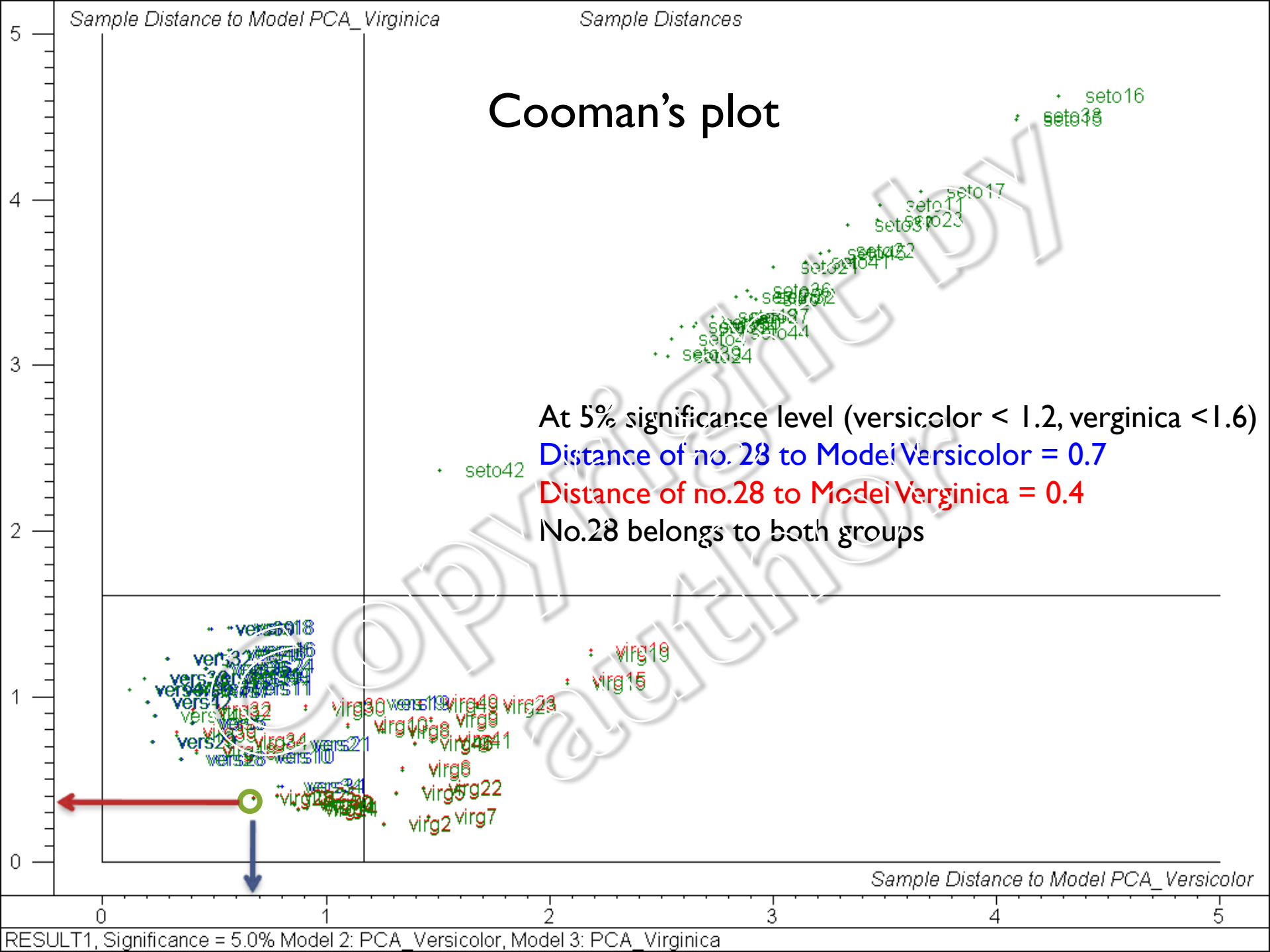
- Cooman's plot
- Model distance
- Discrimination power

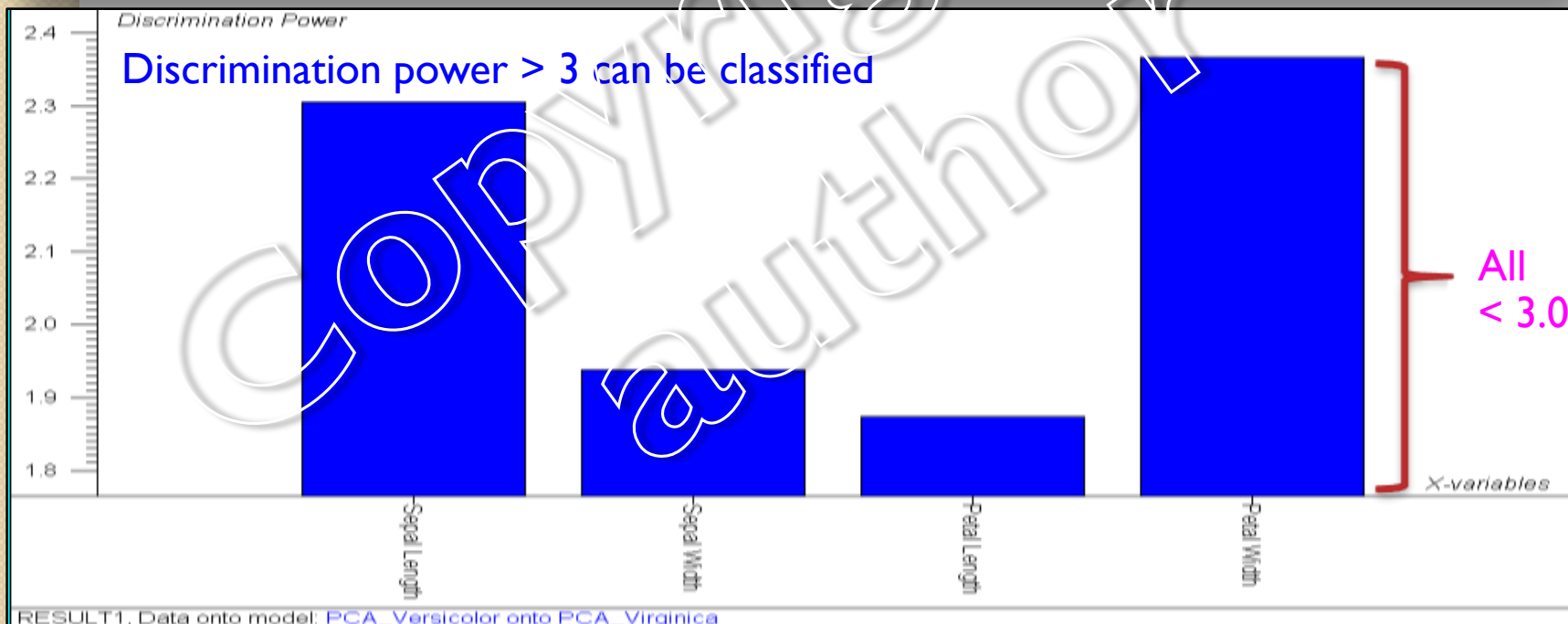
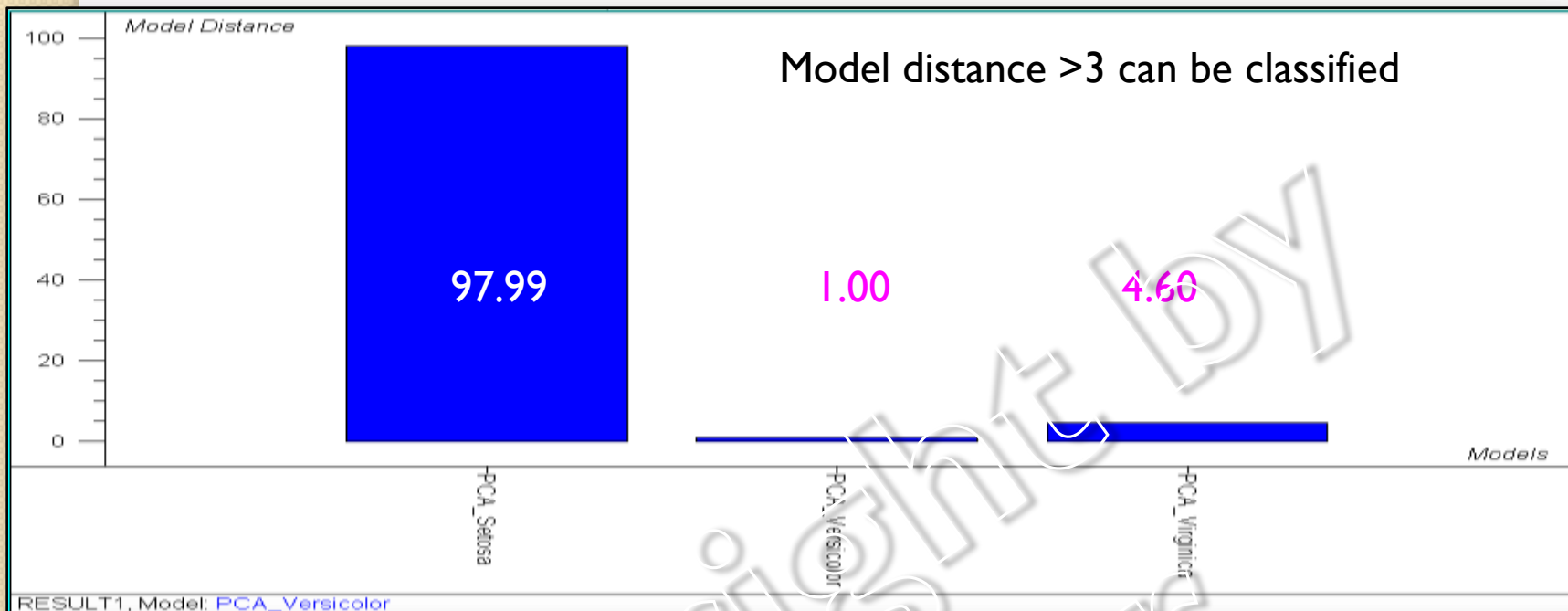
RESULT1, Significance = 5.0%

Sample Distance to Model PCA_Virginica

Sample Distances

Cooman's plot





Thank you for your attention

