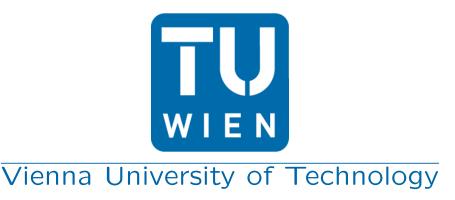
DAS+R: A graphical user interface for multivariate data analysis in R

R. Dutter, A. Zainzinger and A. Alfons Department of Statistics and Probability Theory Vienna University of Technology

Chemometrics Workshop, Vienna June 28, 2010



DAS+R (future package of R)



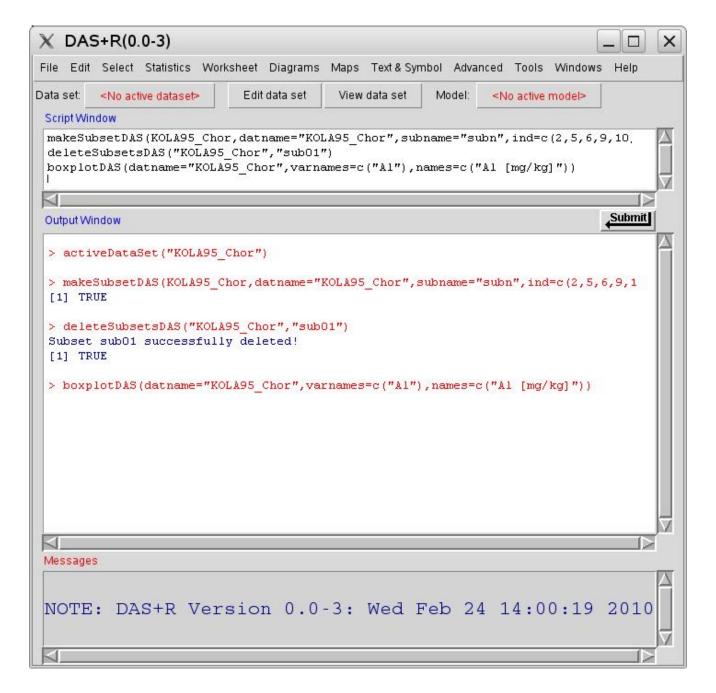
• Basis: DAS, (all) functions of R, Tcl/Tk

• Emphasis:

- easy to use (e.g. Rcommander)
- fast reproducibility (with small changes) of the results
- interactive definition of subsets (numerically and graphically)
- strong interaction between statistical data and spatial information
- graphical analysis

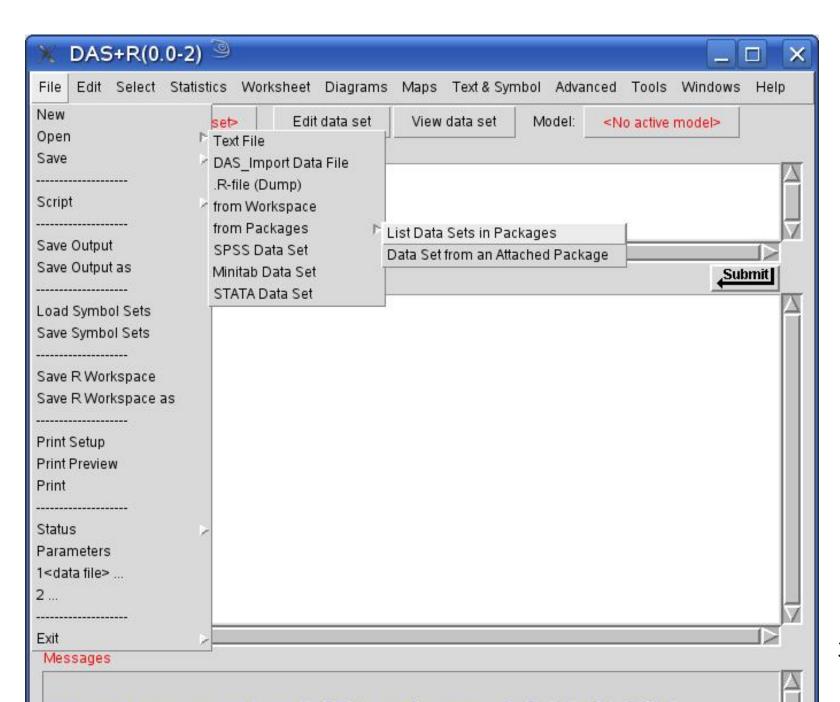






Open Data File





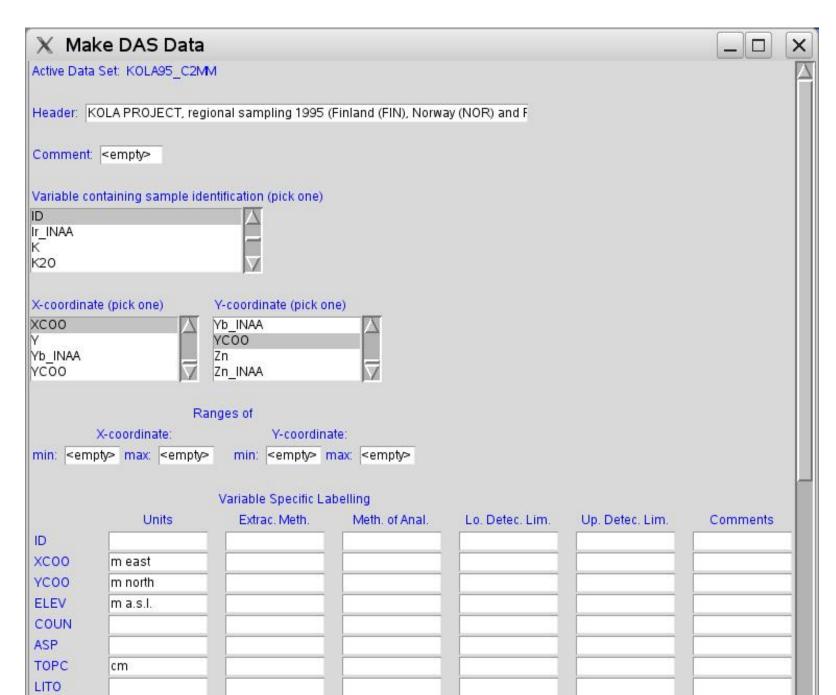
Read DAS/Imp (Preview)



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COMMENT DATASET									C-Horizon of Podsol profiles, air dried, fraction <2 mm
	ID								C TIONZON OT GUSON PROMICS, All MICC, MACHON 42 MINI
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COMMENT VARIABLES									
EXTRACTION									Aqua Regia
METHOD									GF-AAS
UDL									
LDL									0.001
UNIT		m east	m north	m a.s.l.			cm		mg/kg
VARIABLE	ID	XC00	YC00	ELEV	COUN	ASP	TOPC	LITO	Ag
			7693790		FIN	NW		20	0.01
			7679170		RUS	SW		4	0.01
	3		7668150		FIN	N	52	31	0.021
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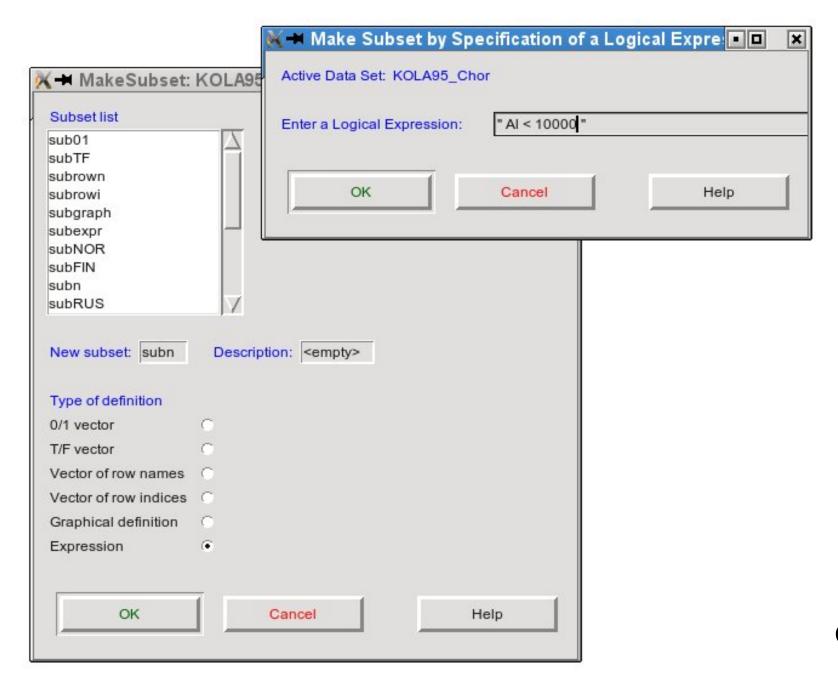
Make DAS Data





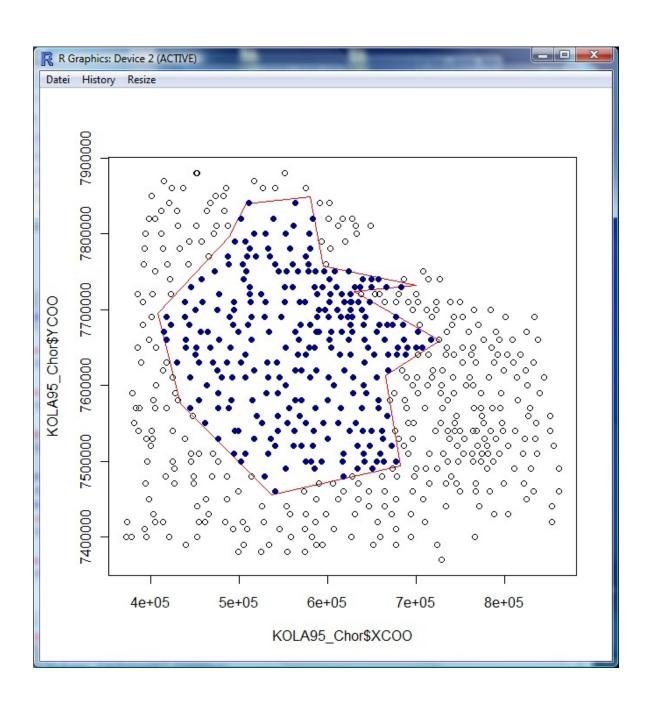
Make Subset: Formula





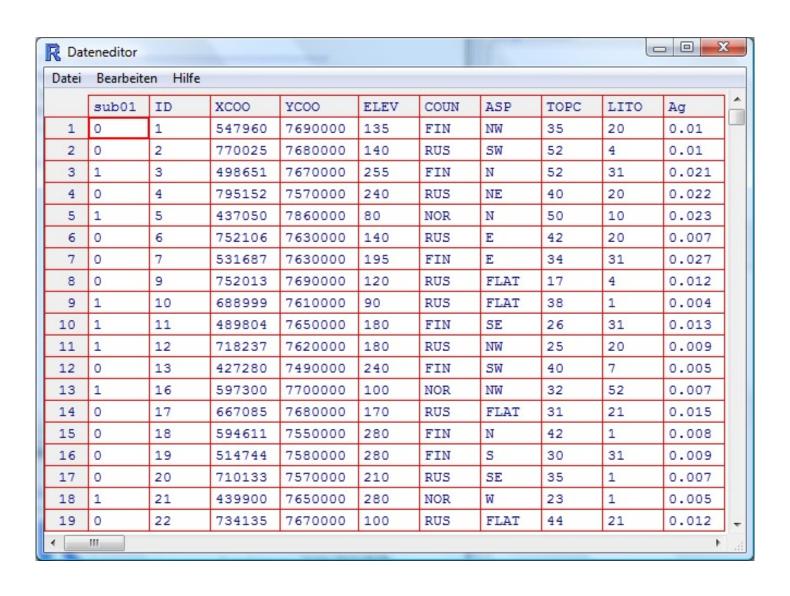
Make Subset: Graphical definition





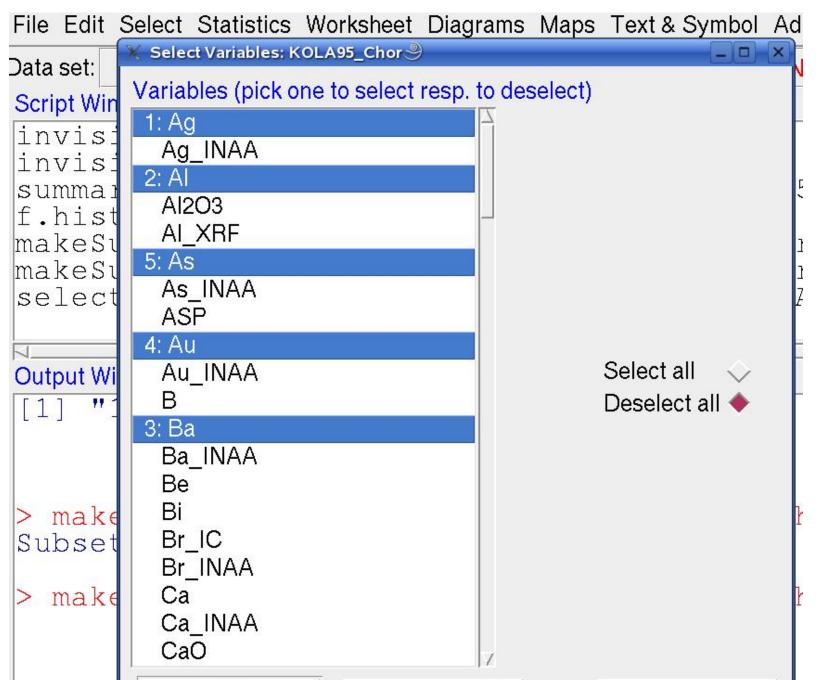
Make Subset: Data editor





(Pre-)Select Variables





View Data Set



- Numerically
- Graphically
 - Boxplot
 - Density Trace
 - Xy-plot
 - Ternary Plot
 - Histogram
 - Scattermatrix (Draftman)

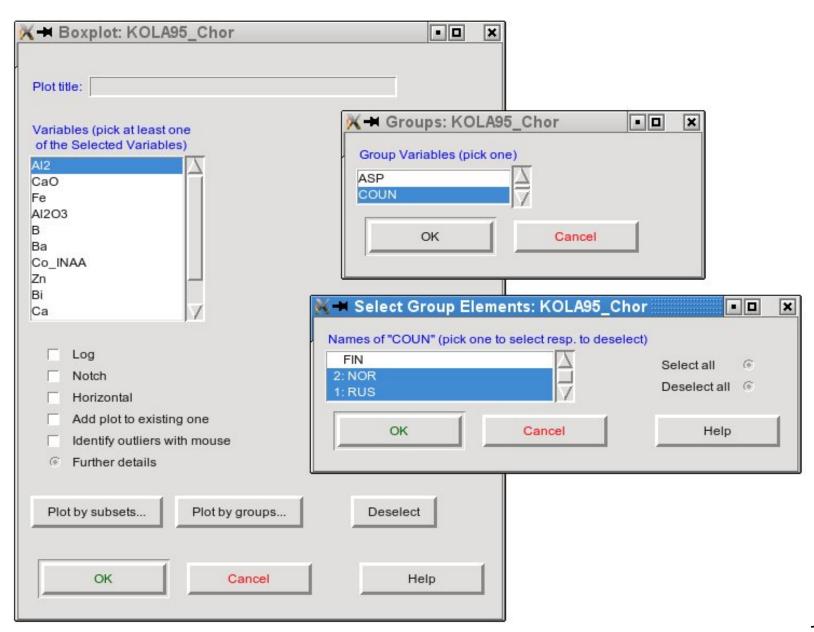
View Data Set



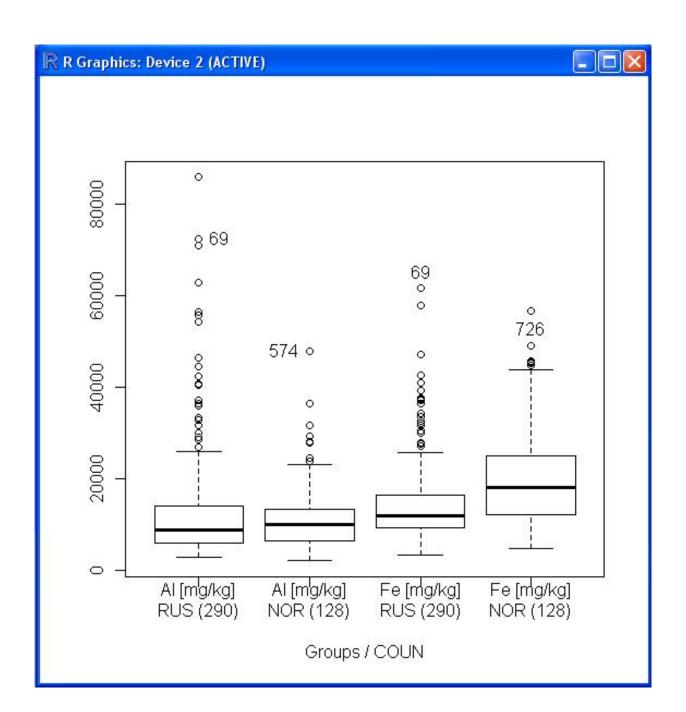
X	9									×
						Г	ору	Paste		Quit
	ID	xcoo	YCOO	ELEV	COUN	ASP	TOPC	LITO	Ag	Ag_INAA
1	1	547960	7690000	135	FIN	NW	35	20	0.01	2.5
2	2	770025	7680000	140	RUS	SW	52	4	0.01	2.5
3	3	498651	7670000	255	FIN	N	52	31	0.021	2.5
4	4	795152	7570000	240	RUS	NE	40	20	0.022	2.5
5	5	437050	7860000	80	NOR	N	50	10	0.023	2.5
6	6	752106	7630000	140	RUS	E	42	20	0.007	2.5
7	7	531687	7630000	195	FIN	E	34	31	0.027	2.5
8	9	752013	7690000	120	RUS	FLAT	17	4	0.012	2.5
9	10	688999	7610000	90	RUS	FLAT	38	1	0.004	2.5
10	11	489804	7650000	180	FIN	SE	26	31	0.013	2.5
11	12	718237	7620000	180	RUS	NW	25	20	0.009	2.5
12	13	427280	7490000	240	FIN	SW	40	7	0.005	2.5
13	16	597300	7700000	100	NOR	NW	32	52	0.007	2.5
14	17	667085	7680000	170	RUS	FLAT	31	21	0.015	2.5
15	18	594611	7550000	280	FIN	N	42	1	0.008	2.5
16	19	514744	7580000	280	FIN	S	30	31	0.009	2.5
17	20	710133	7570000	210	RUS	SE	35	1	0.007	2.5
18	21	439900	7650000	280	NOR	W	23	1	0.005	2.5
19	22	734135	7670000	100	RUS	FLAT	44	21	0.012	2.5
20	23	787098	7500000	140	RUS	FLAT	45	1	0.007	2.5
21	24	624400	7540000	160	RUS	FLAT	41	51	0.008	2.5
22	25	627700	7480000	280	RUS	FLAT	NA	1	0.007	2.5
23	26	386646	7540000	300	FIN	S	36	1	0.004	2.5
24	27	713892	7740000	160	RUS	SW	30	9	0.01	2.5
25	28	579500	7650000	110	RUS	FLAT	32	20	0.011	2.5

Boxplot





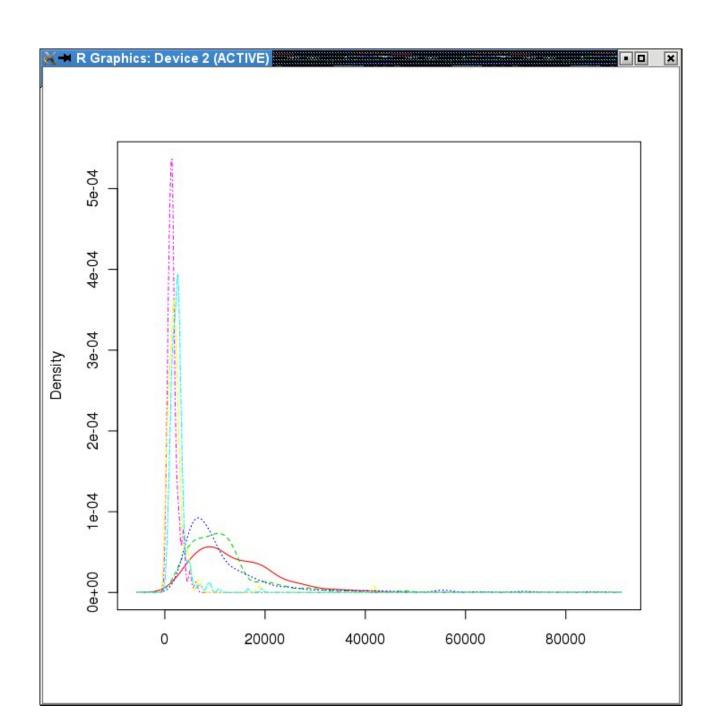




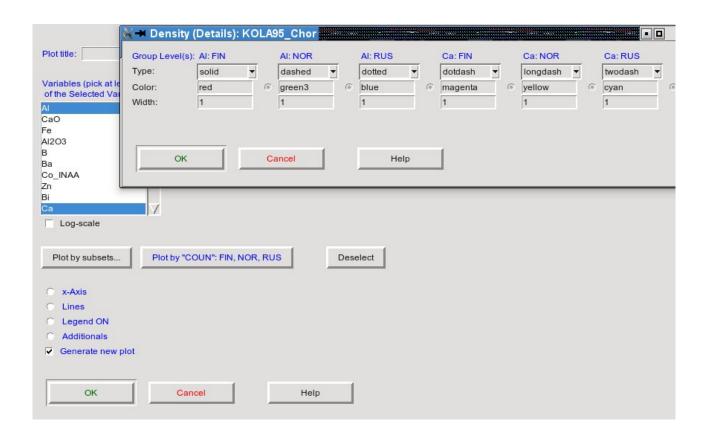


Plot title: Variables (pick at least or of the Selected Variables			
AI CaO Fe AI2O3 B Ba Co_INAA Zn Bi Ca	X V		
Plot by subsets	Plot by "COUN": FIN, NOR, R	us	Deselect
 x-Axis Lines Legend ON Additionals Generate new plot 			
ОК	Cancel	Help	р

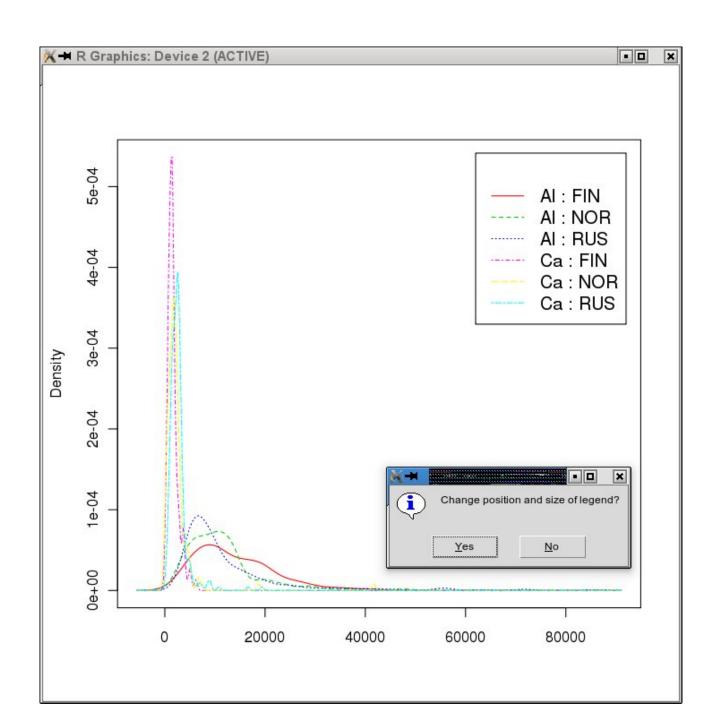










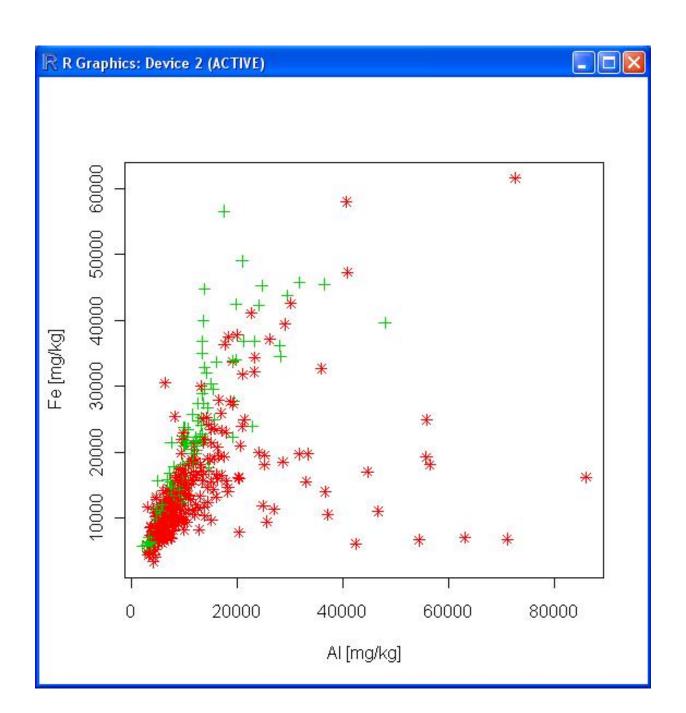




X-variable (pick one	Y-variable (pick one	
of the Selected Variables)	of the Selected Variables)	
AI2	Al2	7
CaO	CaO T	1
e	Fe	
AI2O3	Al2O3	
3	В	
3a	Ba	
Co_INAA	Co_INAA	
Zn —	J Zn L	
3i	Bi	
Ca	Ca	7
	☐ Log-scale	
	Plot by "COUN": RUS, NOR	Deselect
		Deselect
Plot by subsets		Deselect
Plot by subsets F		Deselect
Plot by subsets F		Deselect
Plot by subsets F x-Axis y-Axis Symbols		Deselect
Plot by subsets F x-Axis y-Axis Symbols Legend OFF		Deselect

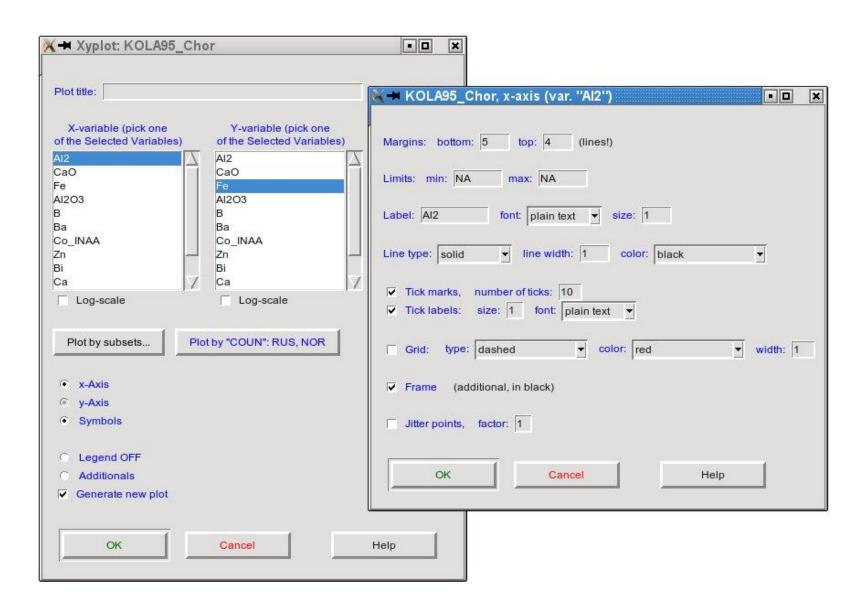






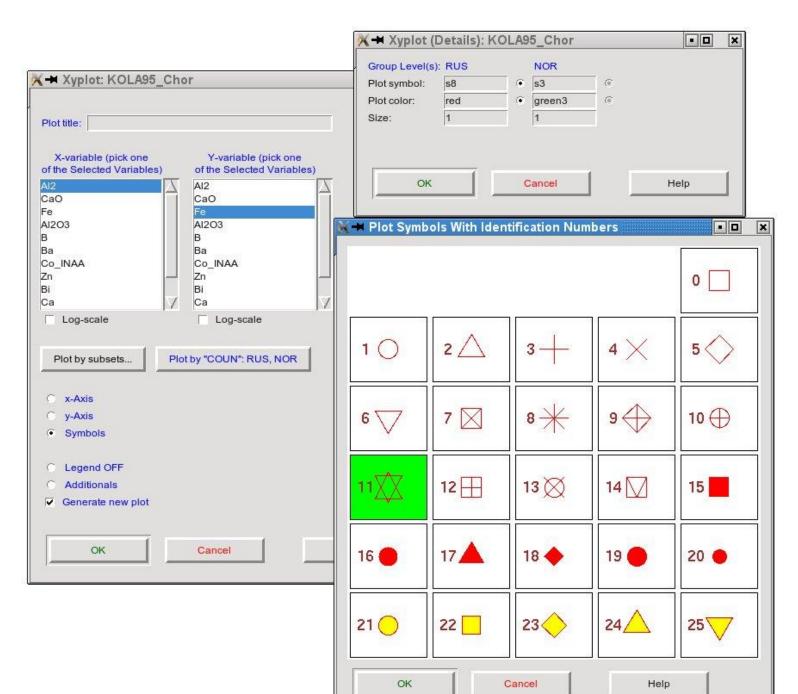
Xyplot: Specifications



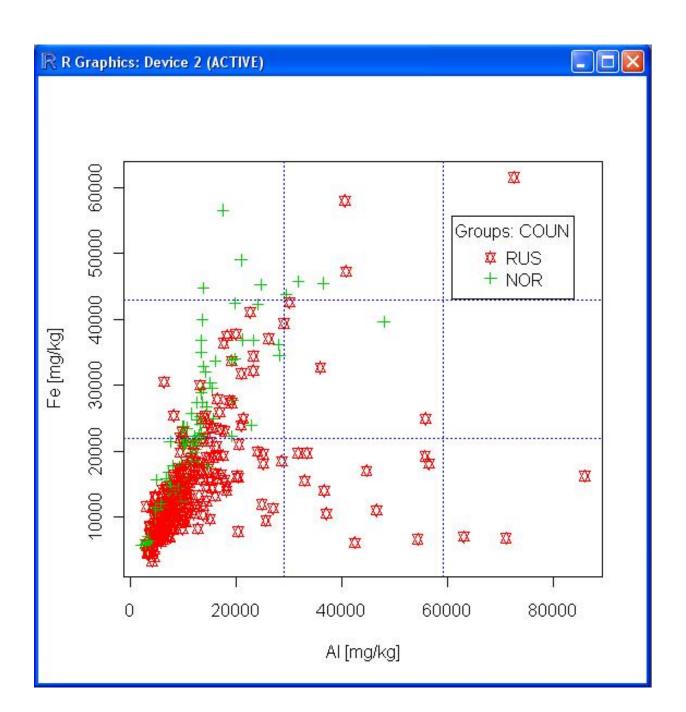


Xyplot: Specifications



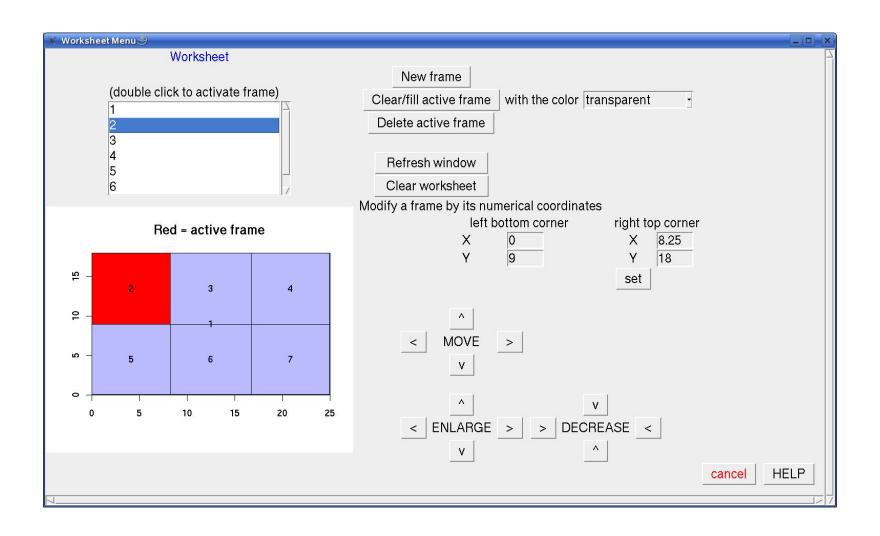






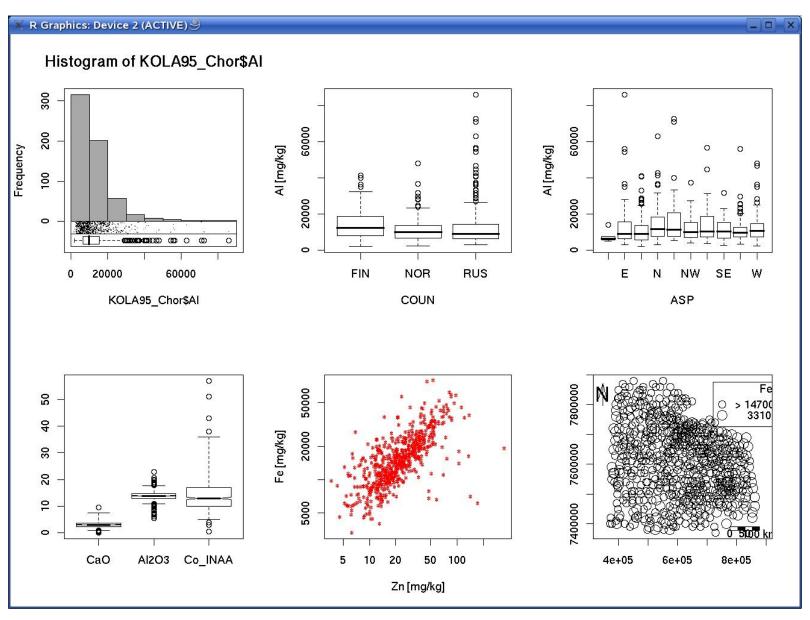
Worksheet Menu





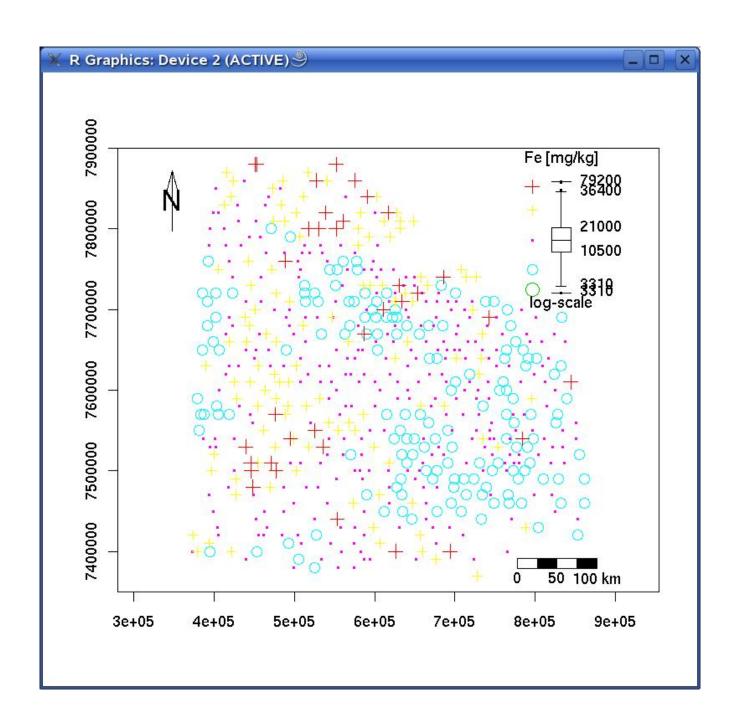
Filled Worksheet





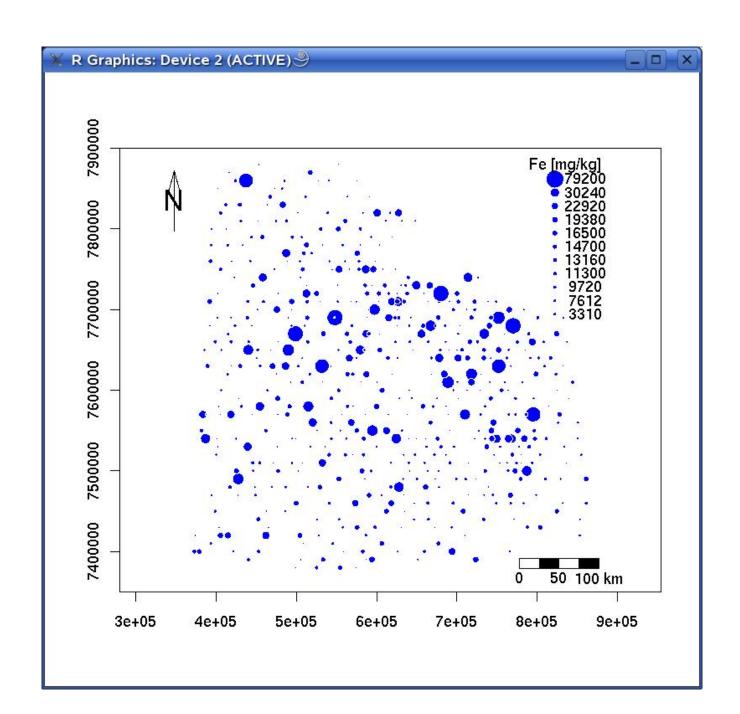
Mapping: Boxplot





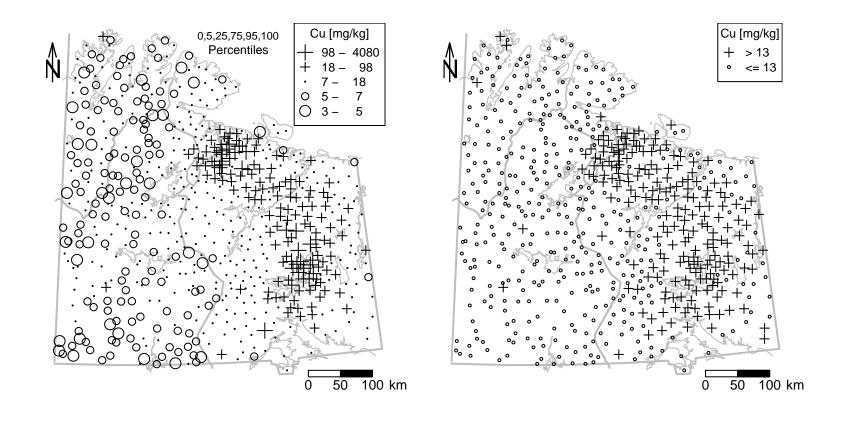
Mapping: Proportional Plot



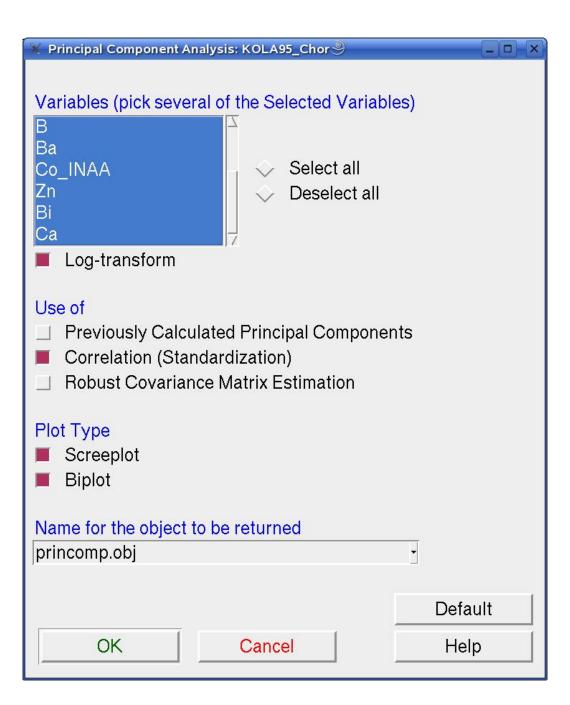


Mapping: Using Background Maps









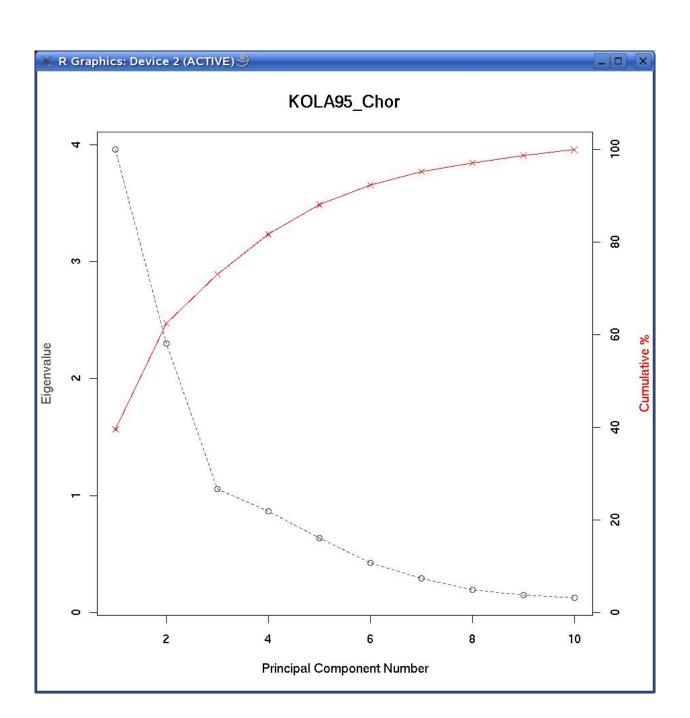


```
Output Window
> princomp.obj <- princompDAS(data=KOLA95 Chor, vars=c("Al", "CaO", "Fe", "Al2O3", "
> summary(princomp.obj)
Importance of components:
                                        PC2
                       1.9886845 1.5158522 1.0274942 0.9298833 0.79809531
Standard deviation
Proportion of Variance 0.3954866 0.2297808 0.1055744 0.0864683 0.06369561
Cumulative Proportion 0.3954866 0.6252674 0.7308418 0.8173101 0.88100572
                                                     PC8
                               PC6
                                          PC7
                                                                PC9
                       0.65051344 0.53951065 0.44207959 0.38933541 0.35872949
Standard deviation
Proportion of Variance 0.04231677 0.02910717 0.01954344 0.01515821 0.01286868
Cumulative Proportion 0.92332250 0.95242967 0.97197311 0.98713132 1.00000000
```



※ Screeplot: KOLA95_Chor◎							
	_A95_Chor cipal Component Number						
Eigenvalues Detai Axis Label: Plot Color: Plot Symbol: Plot Symbol Size: Line Type: Line Width:	Eigenvalue gray32						
Cumulative % Det Axis Label: Plot Color: Plot Symbol: Plot Symbol Size: Line Type: Line Width:	Cumulative % red						
OK	Default Cancel Help						

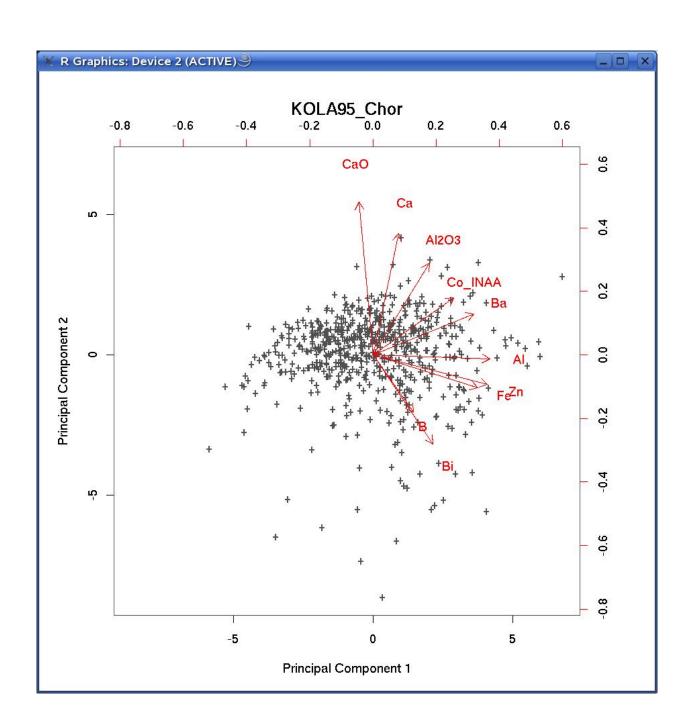






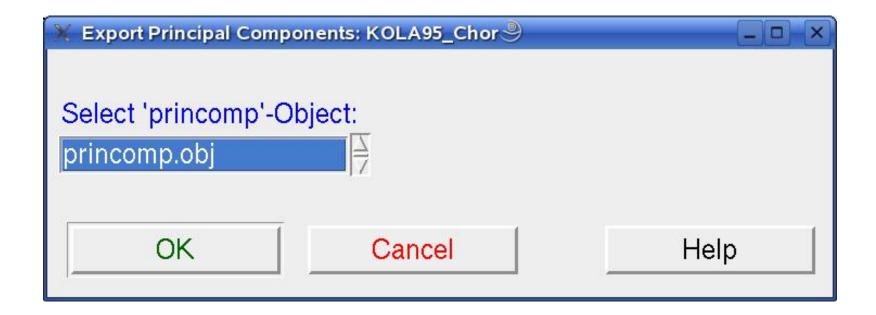
💥 Biplot: KOLA95_Chor🍭	_
Plot Title: KOLA95_	Chor
X-variable (pick one) PC1 PC2 PC3 PC4 PC5	Y-variable (pick one) PC2 PC3 PC4 PC5 PC6
Scores Details Plot Color: Plot String: Plot String Size:	gray32
Loadings Details Arrow Color: Arrow Head Length: Plot Symbol Size:	red (click for 'Select Color' menu) 0.1 1
OK	Default Cancel Help











Summary



- DAS+R is user friendly
- enables to construct complicated R-commands via the GUI
- high repeatability (fast prototyping)
- using of subsets (of variables/observations)
- emphasis on graphical analysis.

 Finally: Embedding of new functions should not be difficult!!!!

Summary

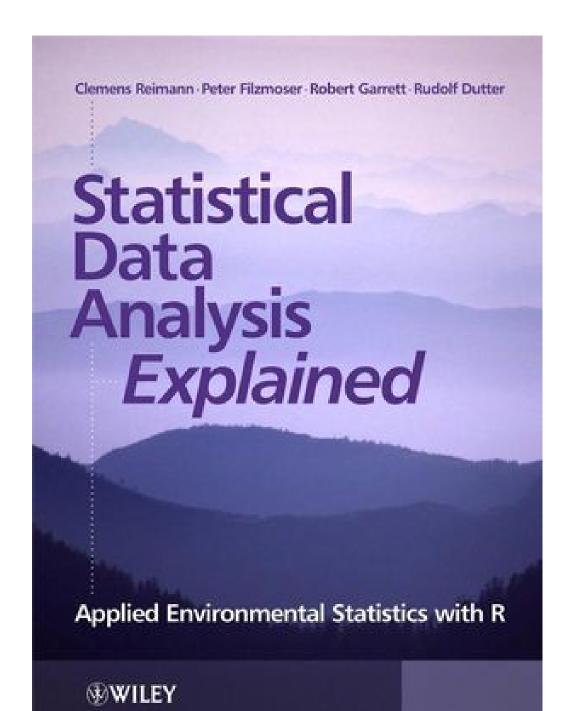


• See

http://www.statistik.tuwien.ac.at/StatDA/DASplusR

Book: Applied Statistical Data Analysis





DAS+R a companion of this book (Wiley, 2008).

Emphasis:

- Spatial Data
- Strong Graphical Tools
- Data from Geochemistry
- Little Mathematics
- Provided Software:
 DAS+R