

Det matematisk-naturvitenskapelige fakultet

Health, Safety and Environment (HSE)



KJM3070 Colloquium



Safe Job Analysis (SJA)

- Safe job analysis must be made for all analytical operations representing any danger
 - What can go **wrong**?
 - What can we do to **avoid** this?
 - What can we do to **minimize** the damage?

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Risk assessment: CertoClav 12L Autoclave

What can go wrong	Possible Risk	What can be done to prevent accidents	What can be done to reduce the consequences if an accident should occur
Explosion due to very high pressure inside chamber (above 4,1 bars)*	Burns, blindness, and possible risk of death	Work in the hood Wait enough time at the end of the experiment, so that the pressure has fallen to 0 bars and the temperature is below 80°C. Use gloves to take out the samples. Follow carefully the step by step	Leave the area if accident should occur & contact safety inspector Vidar Blekestad, supervisor Rolf Vogt, Alexander Engebretsen or Christian W. Mohr. Place the burned area under cold water.
Severe burns due to high temperatures (≈121°C)	Burns	procedure for operating the autoclave (instructions given on autoclave) Always consult an experienced user of the instrument for a demonstration before running the instrument for the first time.	If serious accident should occur contact ambulance and medical help (telephone no.: 113)

*The autoclave is setup with safety vents in order to avoid explosions. However the instrument must always be treated with the possibility of safety failure.

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Safety rutines

- <u>HMS0504 Feltsikkerhet</u> should have been taken before the fieldwork ;-)
- <u>HMS0503 Laboratoriesikkerhet</u> <u>must</u> be taken before the lab work
- In the lab you must use **goggles**
- The doors to chemicals must be **locked**
 - Door to lab must be locked
 - Cabinets must be **locked** and key hidden

Health Safety and Environment

- All participants need to fill in field card form for participants
 - <u>https://nettskjema.no/a/130224#/page/1</u>
 - Responsible of the field: Rolf D. Vogt
 - Project name or course number: KJM3070
 - Start/ Starting date of the field work: 23.10.2020
 - Finishing date of the field work: 23.10.2020
- Participation is mandatory
 - though send me an e-mail and explain why if it is impossible within 2 days



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Analysis plan



Colloquium, KJM3070

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Lab work

Conductivity

- Conductivity meter
 - The instrument is calibrated using 84 µS/cm calibration solutions
- The measurements are done for quality control purposes in order to compare measured and calculated conductivity
- Determined as described in ISO7888 using non-filtered water sample and preferably measured at 25°C.
- The reading is presented as mS m⁻¹ (1mS m⁻¹ = 10µS/cm)
- No SJA needed



{H+} determined using pH electrode

- Orion pH-meter with a Ross pH electrode
 - The pH-meter is calibrated with pH = 4.00 and 7.01 buffer solutions
- Risk of degassing of CO₂
 - Stir till stable wait till stable
- Determined as described in ISO10523 using non-filtered water sample
- Measurements should preferably be conducted at 25°C
- No SJA needed



Total Alkalinity titration

- Determined potentiometrically as described in ISO9963
- Titration with acid to pH 4,5 and preferably measured at 25°C
 CO₃²⁻+ HCO₃⁻ + 3H₃O⁺ ⇒ 2H₂CO₃+ 3H₂O
- Total alkalinity (=[HCO₃⁻]+2[CO₃²⁻]) + H⁺ needed to change the pH from sample pH down to pH 4.5 Endpoint in the acid range
- Also other weak acids (A⁻, Al(OH)³⁻ⁿ)



UV-vis

- > Measurement of absorbency scan and @ λ 254, 400 and 600nm
- Absorbency at UV 254 nm is commonly used as a proxy for Dissolved Natural Organic Matter (DNOM)
 - Strongly correlated with TOC due to conjugated double bonds chromophores





Langtjern - absorbency

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- > Measurement of absorbency scan and @ λ 254, 400 and 600nm
- Absorbency at UV 254 nm is commonly used as a proxy for Dissolved Natural Organic Matter (DNOM)
 - Strongly correlated with TOC due to conjugated double bonds chromophores
- Algae absorb light at UV 254 nm, but more than DNOM at VIS 400 nm
- Read SJA







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Analytical Instrument analysis

Major anions to be determined by Ion Chromatograph (IC)

- Principle
 - The sample is injected in a flow of eluent
 - The analyte ions are separated by different degree of binding to the active sites on the ion exchange material
 - Cations are exchanged with H⁺
 - The activity x specific conductivity of the analyte along with H⁺ in the eluent stream are measured by means of a conductometer



Major anions to be determined by Ion Chromatograph (IC)

https://www.youtube.com/watch?v=q3fMqgT1do8



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Major cations to be determined by MP AES

= Microwave Plasma – Atomic Emission Spectrometer



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Major cations to be determined by MP-AES

https://www.youtube.com/watch?v=sRwpw614aPg, 0'59 to 3'22"





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External analysis

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P determination

- Orthophosphate reacts with <u>ammoniummolybdate</u> to a <u>yellow-coloured</u> phosphorousmolybdate acid, that is reduced with ascorbic acid in the presence of antimony to a strongly <u>blue coloured</u> complex
- This colour is measured photometrically as described in Norwegian Standard (NS 4724)



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Total organic carbon

- High temperature (680°C) catalytic combustion analysis on a Shimadzu TOC instrument
- Principle:
 - The organic carbon is combusted to CO₂ by high temperature and catalysis. The amount of CO₂ produced is measured using an IR detector





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Total organic carbon

• Analytes measured may include:



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Total nitrogen

- Total Nitrogen couples the Shimadzu TOC with a chemiluminescent nitrogen detector.
- The combustion tube is packed with a catalyst (platinum on an alumna support) and assembled in a furnace and heated to 720° C.



ĺ	Reaction 1	4NH ₃ + 5O ₂ > 4NO + 6H ₂ O
	Reaction 2	$2(NH_2)_2CO + 5O_2 > 4NO + 4H_2O + CO_2$
	Reaction 3	$NO + O_{_3} > NO_{_2} + O_{_2}$
	Reaction 4	$NO + O_{3} > NO_{2}^{*} + O_{2}$
	Reaction 5	$NO_{2}^{*} > NO_{2}^{} + hv$

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Data assessment

Problems with analysis of major anions and cations in water

- Anions are analysed in filtered raw water
- Cations are analysed in filtered water digested in acid (HNO₃)
 - Colloidal material (<0.45µm) is included in the cation analysis but not in the anion analysis





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Species in natural freshwater

Central equilibriums in natural water samples

KJM3070



Compilation, calculations and QC of data

- After the analysis the data must be:
 - compiled
 - reckoned in terms of equivalent charge and
 - quality controlled by ion balance and agreement between measured and calculated conductivity

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4		Nesøytjernet	20.okt.19	2000	Kalkbergrunn					59°313	54	10°31'12				10,0	
5		Lysakerelva	22.okt.19	2000	Brunt vann					59°57.5	00'	10°37.406				10,0	
6	1	Årungen	23.okt.19	2000	Landbruk, brunt v	vann, høy turbid	itet, høy vannfør	ring		59°42'0	50	10°44'19	11	4		10,0	
7	2	Gjersjøen	23.okt.19	2000	Skogområde, bru	unt vann				59°45'2	94	10°46'439	10	3,0		10,7	
8	3	Kolbotntjernet	23.okt.19	2000	Algete og brunt v	ann				59°48'3	35	10°47'58	14	3		8,9	
9	4	Sværsvann	23.okt.19	2000	Brunt vann					59°49'0	941	10°53'225	20	,3		7,2	
10	5	Østensjøvann	23.okt.19	2000	Næringsrik, mye	fugl, kloakk				59°49'	04	10°53'22	14	3		8,6	
11	6	Solbergvannet	23.okt.19	2000	Organisk jord, br	unt vann				59°54'(04	10°51'95	14	,1		7,6	
12	7	Lutvann	23.okt.19	2000	Skog, lite nedbør	sfelt, klart vann				59°55'1	19	10°52'62	24	9		9.7	
13	8	Maridalsvannet	23 okt 19	2000	Klart vann råvan	nskilde				59°58'(09	10°47'06	12	3		97	
14	9	Akerselva	23 okt 19	2000	Klart vann, Lirbar	nt			-	59054	79	10°45'44	15	6		10.0	

EXAMPLE 1.3: Estimating the reliability of water analyses Your laboratory returns the following water analysis:

pH = 8.22 $EC = 290 \,\mu\text{S/cm}$

Na⁺ K+ Mg²⁺ Ca²⁺ Cl SO_4^{2-} HCO₃ NO_3^- 13.7 1.18 3.2 42.5 31.2 79.9 39 1.3 mg/l

Is this a reliable analysis?

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Activity

- $\{X\} = \gamma_X \cdot [X]$
 - $\{X\}$ is the activity to X
 - [X] is the concentration to X
 - γ_X is the activity coefficient to X
 - γ_X is dimensionless
 - It is determined by:
 - The diameter (å) of the hydrated X
 - Its valence (n_x)
 - The ionic strength (I)



• when I $\rightarrow 0 \gamma \rightarrow 1$ when I<10⁻⁵M $\gamma \approx 1$

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Activity

$$I = \mu = \frac{1}{2} ([A]n_A^2 + [B]n_B^2 + [C]n_C^2 + \dots) = \frac{1}{2} \sum [X]n_X^2$$

"I" is expressed in mol/L

Molar of the salt give rise to an I equals:

AgCI:	$\frac{1}{2}(c \cdot 1^2 + c \cdot 1^2) = \frac{1}{2} \cdot 2c = 1c$
Ba(IO ₃) ₂ :	$\frac{1}{2}(c \cdot 2^2 + 2c \cdot 1^2) = \frac{1}{2} \cdot 6c = 3c$
BaSO ₄ :	$\frac{1}{2}(c \cdot 2^2 + c \cdot 2^2) = \frac{1}{2} \cdot 8c = 4c$
AI(NO ₃) ₃ :	$\frac{1}{2}(c \cdot 3^2 + 3c \cdot 1^2) = \frac{1}{2} \cdot 12c = 6c$

I can be roughly estimated based on the amount of solved material (TDS): I = $2.5 \cdot 10^{-5} \cdot TDS (mg/L)$ UiO *** Kjemisk institutt** Det matematisk-naturvitenskapelige fakultet

Debye Huckel (DH) equation

• For ionic strengths (I) < 0.1 M the γ_X can be calculated by means of the e.g. *Debye Huckel* equation:

$$| < 0.1 \text{ M} - \log \gamma_x = 0.5 n_x^2 \frac{\sqrt{I}}{(1 + 0.33 a_x^2 \sqrt{I})}$$

I < 0.005 M

 $(1+0.33a_x\sqrt{0.005}) \approx 1$

$$-\log \gamma x = 0.5 n x^2 \sqrt{I}$$

- 0.5 & 0.33 are temperature dependent table values
 - Presented values are for 25° C
- å_X is a table value for the specie in question



Species	å
H_3O^+	9
$Na(H_2O)_6^+$	4
$K(H_2O)_6^+$	3
$Cl(H_2O)_6$	3
$Mg(H_2O)_6^{2+}$	8
$Ca(H_2O)_6^{2+}$	6
$Ni(H_2O)_6^{2+}$	6
$Cu(H_2O)_4^+$	6
$Zn(H_2O)_4^{2+}$	6
$Pb(H_2O)_6^{2+}$	5
$Al(H_2O)_6^{2+}$	9
$Fe(H_2O)_6^{2+}$	9

Calculated vs. Measured conductivity

• Calculate:

 $\mu M \to \mu eq/L$

Ionic strength (I)

Activity {x}

Specific conductivity $\rightarrow SC_X = \Lambda^0_m \gamma_X m$

Add all the specific conductivities

Compare measured with specific conductivity





Statistical analysis

- Correlation matrix
 - Identify parameters that are directly correlated or co-variate cell apr

d)

02

												ı	PH Hittide PH Hittide PH F - C C 2 PH F - C	1
	H± k	el IV-a	SAD	DOC	Co2+	Ma2+	No+	1/-	SO42	NO3	CL F			
sUVa	0,806	50 V a	JAN	DOC	Cazi	ivigz i	INGI	N.	0042-	1103-		1661 04	[*] pH • • • • • • • • • • • • • • • • • • •	
	0,000													0.75
													r_CO2	0.75
SAR	0,772	0,852											r_CO2_cell	
	0,000	0,000												
DOC	0,842	0,867	0,953										N2 O O	0.5
	0,000	0,000	0,000										r_CH4	
0-21	0.204	0.177	0.046	0.100	2								r_N2O	
Cazt	-0,301	-0,177	-0,046	0.381	2 									
	0,002	-,												0.25
Mg2+	-0,434	-0,344	-0,254	-0,322	2 0,93	4							r_N2	
	0,004	0,026	0,105	0,038	3 0,000)								
Na+	-0.265	-0 179	-0.062	-0.158	0.81	5 0.822	,							_
	0,090	0,256	0,698	0,327	7 0,000	0,000	-							0
													N2O	
K+	-0,234	-0,140	-0,031	-0,048	3 0,83	4 0,832	2 0,815							
	0,136	0,378	0,045	0,76	0,000	J U,UUL	0,000							0.25
SO42-	0,365	0,587	0,716	0,641	0,42	5 0,239	0,444	0,450						0.25
	0,017	0,000	0,000	0,000	0,00	5 0,128	3 0,003	0,003						
NOD	0.040	0.4.40	0.440	0.40	0.00		0.470	0.004	0.400				TN	
NU3-	-0,246	-0,140	-0,143	0,10 0,308	I U,36 3 0.011	1 0,538 3 0,000	0,476	0,621	0,166					-0.5
	0,110	0,010	0,000	. 0,000	0,01	0,000	, 0,001	0,000	0,200				C	
CI-	-0,456	-0,405	-0,316	-0,393	3 0,69	1 0,764	0,931	0,749	0,213	0,542			FC	
	0,002	800,0	0,041	0,010	0,00	0,000	0,000	0,000	0,176	0,000			Br	
Free PO4	0.356	0.647	0.576	Π 4 79	3 D.D.43	7 -0.086	6 0.024	0.005	0.655	0.072	-0.186		CH4	0.75
	0,021	0,000	0,000	0,001	0,04	0,586	0,873	0,973	0,000	0,651	0,238		CH4 CO2	
													Cells	
нсоз	-0,500	-0,445	-0,377	-0,431	0,84	1 0,846	0,608	0,607	0,023	0,222	0,600	-0,202		
	0,001	0,003	0,014	0,004	+ 0,000	u UUU) U,UUU	0,000	0,883	0,158	0,000	0,199		-1

Multivariate statistics

 How to interpret information in a data matrix of 1000 samples with typically 20 – 30 parameters

	٨	В	С	D	E	F	G	Н	I	J	K	L	H	N	0	P	Q	R	S	Т	U	V	97	Х	Y
1	TieShanPing		Week/		Sampling			If pH>5.0			DOC	Colour													
2	Log	Plot	Lysimeter	Туре	Date	Volume		Alkalinity	Cond _{25C}	Temp.	OD _{254nm}	OD _{410nm}	Ali	Alo	Ca ²⁺	Mg ²⁺	Na ⁺	K*	NH4 ⁺ -N	SO42.S	NO ₃ '-N	CI.	Tot-F	Tot-N	Tot-P
3	Number	Letter	Number		dd.mm.vv	ml	nН	mmol 1 ⁻¹	mS m ⁻¹	°C	Abs cm ⁻¹	ma Pt I ⁻¹	mg ALL-1	mg ALL-1	mg 1 ⁻¹	mg 1-1	mg 1-1	mg 1-1	mg N1-1	mg S1-1	mg N 1-1	mg 1-1	mg 1-1	mg N1-1	ma P I ⁻¹
46	274	4	Tuniou	CTF	16.apr.01	1280,0	4,55	innor c	17,0	25,0	0,224	13,00	910	110	12,23	1,84	0,53	6,45	2,42	17,07	1,02	2,87	0,50	4,08	10,00
47	359	4		CTF	14.mai.01	2410.0	5,22		11,7	25,0	0,182	11,40	220	130	6,05	1,08	0,21	5,27	3,73	10,85	0,81	2,11	0,22	5,49	10,00
48	444	4		CTF	11.jun.01	4200,0	4,51		10,3	25,0	0,169	9,80	460	80	5,37	0,75	0,09	3,46	2,28	9,60	0,73	1,15	0,16	3,93	31,00
49	529	4		CTF	09.jul.01	1170,0	4,15		18,9	25,0	0,274	15,10	1055	165	10,98	1,88	0,11	8,09	3,39	18,60	0,75	2,50	0,35	4,61	5,00
50	699	4		CTF	03.sep.01	1660,0	4,48		18,8	25,0	0,322	20,70	1110	240	15,29	2,24	0,30	7,33	4,27	20,69	1,28	3,49	0,38	5,95	18,00
51	784	4		CIF	01.okt.01	1410,0	4,92		18,9	25,0	0,267	19,80	810	230	14,93	1,42	0,11	6,27	3,86	21,00	1,02	2,62	0,43	5,04	12,00
52	869	4		CIF	29.0kt.01	2580,0	3,97		18,2	25,0	0,204	12,40	2920	F 40	13,20	1,43	0,67	5,98	2,38	17,76	0,90	3,01	0,38	1,91	8,00
54	1039	7		CTE	20.nov.01	1230.0	3,50		45,0	25,0	1 018	58.20	1680	250	10.50	2,50	0.03	9.90	4,02	40,13	1.42	4.49	0.64	2.81	6.00
55	191	5		CTE	19 mar 01	590.0	4 31		20,5	25,0	0.385	22 30	1580	250	20.90	2,13	1 13	10.04	3.66	24.53	2.49	3,78	0.82	7.55	10.00
56	276	5		CTF	16.apr.01	1590.0	4.72		11.9	25.0	0.33	15.80	460	80	9.68	1.66	0.92	5.13	2.17	11.55	0.70	2.00	0.35	2.76	6.00
57	361	5		CTF	14.mai.01	3050.0	4.83		8.8	25.0	0,149	9.00	340	0	4.25	0.82	0.16	3.69	2.25	7.37	0.60	1.39	0.21	2.92	4.00
58	446	5		CTF	11.jun.01	4750,0	4,64		6,8	25,0	0,145	9,00	320	50	3,52	0,66	0,06	2,56	1,28	5,70	0,46	0,87	0,09	2,21	41,00
59	531	5		CTF	09.jul.01	1400,0	4,13		13,8	25,0	0,209	10,30	876	84	6,84	1,33	0,08	5,29	2,09	13,11	0,50	1,66	0,21	3,03	2,00
60	701	5		CTF	03.sep.01	1610,0	5,48		13,7	25,0	0,236	16,10	450	160	9,89	1,29	0,29	5,88	4,08	14,55	0,86	2,84	0,34	5,66	28,00
61	786	5		CTF	01.okt.01	1380,0	4,18		15,4	25,0	0,167	8,30	910	90	9,82	1,17	0,20	4,59	2,96	14,77	0,85	2,05	0,51	3,89	7,00
62	871	5		CTF	29.okt.01	3230,0	3,76		12,9	25,0	0,122	4,90	480	420	5,15	0,85	0,36	3,15	1,22	9,49	0,63	2,03	0,22	1,91	2,00
63	956	5		CIF	26.nov.01	830,0	3,41		34,5	25,0	0,252	8,90	2090	220	19,48	1,66	0,56	5,99	2,77	27,53	2,19	3,77	1,14	4,81	6,00
65	1041	5		CIF	24.des.01	1040,0	3,49		23,9	25,0	0,183	7,10	1160	100	7,23	0,95	0,17	4,00	1,35	14,73	1,26	2,65	0,47	2,68	9,00
65	195	6		CTE	19.mar.01	1676.0	3,01		46,3	25,0	0,495	24,70	740	250	12.50	3,19	1,39	7,95 E 47	0,02	35,40	3,15	5,10	1,00	0,90	40,00
67	260	6		CTE	14 mai 01	3560.0	4.01		13.8	25,0	0,266	11.50	450	160	6.16	0.92	0.21	3.09	2,40	10.72	0,76	2,50	0,45	3,57	6,00
68	450	é		CTE	11 iun 01	5220.0	4.02		11.9	25.0	0.189	10.00	380	40	4 21	0.70	0.41	3 33	2.28	9.56	0,05	1.54	0.17	3.52	49.00
69	535	ĕ		CTF	09.jul.01	1540.0	3.62		25.4	25.0	0.225	10.30	1320	110	10.51	1.64	0.18	4.65	4.68	20.71	0.96	2.33	0.40	6.00	17.00
70	620	6		CTF	06.aug.01	3390.0	5.30		10.9	25.0	0.292	21.80	380	120	6.74	0.98	0.09	3.85	2.51	9.41	0.82	2.61	0.30	5.10	8.00
71	705	6		CTF	03.sep.01	1590,0	3,69		28,7	25,0	0,352	17,80	1400	150	17,83	2,26	0,37	5,65	4,95	25,79	1,42	3,65	0,51	6,87	16,00
72	790	6		CTF	01.okt.01	1380,0	3,72		31,1	25,0	0,237	16,00	1580	130	20,10	2,26	0,29	4,83	6,38	31,35	1,44	3,46	0,70	8,59	12,00
73	875	6		CTF	29.okt.01	3070,0	3,30		29,4	25,0	0,216	9,60	1620	100	11,25	1,83	0,64	4,33	2,32	21,69	1,03	3,01	0,42	3,40	5,00
74	960	6		CTF	26.nov.01	520,0	3,00		74,1	25,0	0,396	13,60	4140	400	38,60	3,59	1,09	10,42	5,00	60,03	3,50	8,19	2,15	8,81	16,00
75	1045	6		CTF	24.des.01	1180,0	3,26		36,5	25,0	0,22	6,80	1610	140	10,80	1,63	0,45	6,15	1,45	25,83	1,28	3,46	0,57	2,66	10,00
76	197	7		CTF	19.mar.01	450,0	3,69		34,4	25,0	0,58	30,50	2470	330	39,60	3,80	1,93	14,34	8,58	49,67	4,81	7,73	1,38	17,20	30,00
77	282	1		CIF	16.apr.01	1420,0	3,79		23,6	25,0	0,337	18,40	1200	130	13,09	1,88	0,62	6,66	3,10	27,44	1,04	2,95	0,45	4,60	6,00
70	307	7		CTE	14.mai.01	5550,0	4,00		10,0	25,0	0,25	10,20	400	50	5.24	0,94	0,50	4,00	3,95	12,01	0,94	1,00	0.19	0,22	4,00
80	637	7		CTE	09 int 01	1080.0	3.69		28.6	25.0	0.267	16.70	1850	140	13.60	2.25	0.03	8.09	5.99	26.56	1.11	2.62	0.42	7.44	27.00
	622	7		CTF	06 aug 01	3100.0	5.49		12.2	25.0	0.368	29.80	390	130	6.15	1.09	0.10	5.53	2.95	9.83	0.78	2.39	0.39	5.99	3 00
82	707	7		CTF	03.sep.01	1580.0	3,71		32.9	25.0	0,376	19,40	1620	170	18,40	2.65	0.40	6.38	8,12	29.98	1.77	3.69	0.51	10.31	405.00
83	792	7		CTF	01.okt.01	1540,0	3,98		30,1	25,0	0,358	21,30	1156	114	23,94	2,39	0,28	6,46	6,70	32,55	1,60	3,52	0,60	8,44	18,00
84	877	7		CTF	29.okt.01	2340,0	3,30		23,4	25,0	0,26	12,30	1880	130	13,84	1,80	0,20	6,71	3,31	26,27	1,30	3,39	0,44	4,33	6,00
85	962	7		CTF	26.nov.01	465,0	3,01		79,4	25,0	0,458	19,20	4510	420	44,66	3,91	1,03	15,75	7,37	70,37	4,30	9,40	2,09	11,60	15,00
86	1047	7		CTF	24.des.01	660,0	3,07		62,6	25,0	0,316	10,90	2740	230	21,00	2,59	1,04	10,34	2,05	39,97	2,08	6,12	1,26	4,84	27,00
87																									
00																									
00																									
91	187	A		FTF	19 mar 01	580.0	4.76	erectivity	18.9	25.0	0.271	15.50	970	220	15.82	2.02	0.71	9.13	3.02	19.34	1.61	5.06	0.48	5.38	10.00
92	527	A		FTF	09. jul. 01	840.0	5.01		9.7	25.0	0.201	11.40	350	70	4.54	0.94	0.03	3.37	2.47	9.34	0.62	1.27	0.13	4.01	69.00
93	697	A		FTF	03.sep.01	880.0	4,34		19,0	25.0	0,335	18,50	820	120	12,82	1,82	0.22	6.04	4.03	18,63	1.38	2.69	0.35	6,80	17,00
94	782	A		FTF	01.okt.01	1010,0	4,18		18,9	25,0	0,244	12,70	610	40	13,29	1,58	0,14	4,94	4,89	18,96	1,28	2,09	0,40	5,63	56,00
95	867	A		FTF	29.okt.01	2180,0	3,97		15,9	25,0	0,218	12,60	650	340	8,62	1,46	0,25	6,07	2,65	13,83	0,87	2,72	0,26	3,46	79,00
96	952	A		FTF	26.nov.01	490,0	3,49		38,4	25,0	0,31	12,40	2250	160	24,60	2,64	0,57	9,47	4,34	37,40	2,59	6,02	1,41	6,57	11,00
97	1037	A		FTF	24.des.01	960,0	3,71		19,2	25,0	0,202	7,50	840	50	8,49	1,30	0,53	5,42	1,30	13,39	0,98	2,83	0,39	2,37	9,00
98	188	В		FTF	19.mar.01	400,0	3,81		44,0	25,0	0,5	29,90	3150	580	32,88	4,31	1,79	21,50	7,78	45,13	4,74	8,94	1,31	15,20	0,00
4 4	E All data	Statist	ics / Table /	2001 2	002 2001 -	2003 91	/									4		- 00			- 10				

Cluster analysis

Organizing parameters that co-variate

in clusters

- Identify
 - Links between parameters and groups of parameters
 - Identify key explanatory factors
 - General patterns

Cluster analysis



Principal Component Analysis

- Makes an n-dimentioal graph of your n parameters
- Identifies the greatest variation in the swarm of data points and draws the PC1 through its axis.
- Identifies the next PC perpendicular to the previous
- Produce loading plots that are projections of the points to the PC plane



Score Plot of H+; ...; DOP



Det matematisk-naturvitenskapelige fakultet

Szopińska et al., 2016

