

Exam: Computational life science, 15.0 hp
Date: 2009.11.04
Time: 9-15
Place: Skrivsal 3, Östra paviljongen
Contact: Torgeir R. Hvidsten (tel. 5248)

Pocket calculator and dictionary allowed. No other aids (books, notes, etc.). Answers can be given in English or Swedish.

NB: Answer the three tasks on separate paper sheets. This way the three teachers can correct in parallel and you will get the results back faster.

Task 1 (30%) Statistics

a) 10%

An investigator was interested to study how washing affects the strengths of lengths of yarn. The following figures give the strengths for two random samples of lengths of yarn, the first sample being taken before washing and the second after six washings.

Before washing:	12.3	13.7	10.4	11.4	12.9	12.6	
After 6 washings:	15.7	14.3	12.6	14.5	12.6	13.8	11.9

The investigator decided to use the two sided two-sample t-test to test if the washing did have an effect on the extension of the yarn.

1. Formulate a formal hypothesis that is being tested by the experiment.
2. The experiments p-value was 0.0662. What conclusions can you draw from the experiment?

b) 10%

Crocus flowers can have three colors; yellow, purple and white. In order to test for homogeneity (i.e. that the three colors are equally common) a small experiment including 20 flowers was conducted. Eight flowers were yellow, 8 purple and 4 white. Use a chi-square test to test for homogeneity at a 5% critical significance level.

You need to use the chi-square table below to solve the problem.

Degrees of freedom	P = 0.05	P = 0.01	P = 0.001
1	3.84	6.64	10.83
2	5.99	9.21	13.82
3	7.82	11.35	16.27
4	9.49	13.28	18.47
5	11.07	15.09	20.52
6	12.59	16.81	22.46
7	14.07	18.48	24.32
8	15.51	20.09	26.13
9	16.92	21.67	27.88

c) 10%

Cars fuel consumption measured in Gallons per 100 mile (Fuel) can to some degree be explained by the cars weight in kilograms (Weight). Linear regression was used to model the relationship between the response variable Fuel and the explanatory variable Weight. The result of an analysis in R is shown below. Use the information to answer the following questions:

1. Can Weight be used to explain the variable Fuel? Motivate your answer.
2. How much of the variation in the variable Fuel is explained by the model?
3. Use the model to predict the fuel consumption of a car that weights 1800 kg.

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*** Linear Model ***
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Call: lm(formula = Fuel ~ Weight, data = Fuel.data, na.action = na.exclude)
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Residuals:
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      Min       1Q   Median       3Q      Max
-0.7957 -0.2703  0.01414  0.2547  0.9583
```

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Coefficients:
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              Value Std. Error t value Pr(>|t|)
(Intercept)  0.3914   0.2995     1.3070  0.1964
Weight       0.0013   0.0001    12.9323  0.0000
```

```
Residual standard error: 0.3877 on 58 degrees of freedom
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```
Multiple R-Squared: 0.7425
```

```
F-statistic: 167.2 on 1 and 58 degrees of freedom, the p-value is 0
Multiple R-Squared: 0.7425
```

```
F-statistic: 167.2 on 1 and 58 degrees of freedom, the p-value is 0
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Task 2 (35%) Bioinformatics

a) (10%) Perl and programming

1. What is the difference between an array and a hash in Perl?
2. Write Perl programs that determine the number of unique elements in a list, e.g.

Input: (1,2,3,3,4,5), Output: 5

Input: (a,a,a,b,c), Output: 3

Write two programs; one that uses arrays and one that uses hashes.

3. What can you say about the time complexity of your two programs?

b) (10%) Sequence alignment

1. Consider the following scoring matrix δ for sequences in a six letter alphabet

	A	B	M	O	S	T	-
A	1	-1	-1	-2	-2	-3	-1
B		1	-1	-1	-2	-2	-1
M			2	-1	-1	-2	-1
O				1	-1	-1	-1
S					1	-1	-1
T						2	-1
-							-1

and the two sequences:

$v = \text{MOAT}$

$w = \text{BOAST}$

Fill out the dynamic programming table for a *global* alignment between v and w under the scoring matrix δ . Draw arrows in the cells to store the backtrack information. What is the score for the optimal alignment and what alignment(s) does this score correspond to?

2. *Blast* provides the user with an E-score for each pair-wise alignment. What is the interpretation of this score? How is it computed?

c) (5%) Phylogenetic trees

There are two main approaches to construct phylogenetic trees: Distance methods and Discrete data (tree searching) methods. Briefly describe the main principles behind each of the two

methods. Compare the two approaches: what are their main strengths and weaknesses relative to each other?

d) (10%) Machine learning

1. Briefly explain what a decision tree is and how you can infer a decision tree from data (examples). What search strategy (algorithm design technique) does one use to infer decision trees? What is the main advantage and disadvantage of this search strategy?
2. Explain what we mean by overfitting in the context of inducing models from data using machine learning. Give an example using one machine learning technique. How can one avoid overfitting?

Task 3 (35%) Chemometrics

a) (20%)

You have investigated four factors with 11 experiments based on a fractional factorial design (2^{4-1}) and three center points, and investigated a response y (see table below).

1. What is the resolution of the fractional factorial design?
2. Calculate the regression model coefficients for: $y = b_0 + b_1X_1 + b_2X_2 + b_3X_3 + b_4X_4$
 - Interpret the results.
3. Calculate R^2 for the model in b).
 - Interpret the results.
4. What are confounded with your main terms?
 - What does this information mean?
5. Calculate the pure error and the model error of your regression model.
 - Use that information to judge the quality of the model. An F table for $\alpha = 0.05$ is given at the last page.

<i>Exp. No.</i>	<i>X1</i>	<i>X2</i>	<i>X3</i>	<i>X4</i>	<i>y</i>
1	-1	-1	-1	-1	2,27
2	1	-1	-1	1	11,44
3	-1	1	-1	1	-2,15
4	1	1	-1	-1	5,09
5	-1	-1	1	1	4,15
6	1	-1	1	-1	9,50
7	-1	1	1	-1	0,59
8	1	1	1	1	5,50
9	0	0	0	0	4,56
10	0	0	0	0	5,45
11	0	0	0	0	5,30

b) (5%)

How do you determine the number of significant components in principal component analysis?

c (10%)

Give explanations, and its usage/importance in design of experiments and/or multivariate analysis of the below listed items.

1. Score and loading plots
2. Random correlation, and correlation vs. causation
3. D-optimal design

F-table for alpha = 0.05: F(0.05,df1,df2)

df2/df1	1	2	3	4	5	6	7	8	9	10	12	15	20	24	30	40	60	120	inf
1	161.4	199.5	215.7	224.6	230.2	234.0	236.8	238.9	240.5	241.9	243.9	245.9	248.0	249.1	250.1	251.1	252.2	253.3	254.3
2	18.51	19.00	19.16	19.25	19.30	19.33	19.35	19.37	19.38	19.40	19.41	19.43	19.45	19.45	19.46	19.47	19.48	19.49	19.50
3	10.13	9.55	9.28	9.12	9.01	8.94	8.89	8.85	8.81	8.79	8.74	8.70	8.66	8.64	8.62	8.59	8.57	8.55	8.53
4	7.71	6.94	6.59	6.39	6.26	6.16	6.09	6.04	6.00	5.96	5.91	5.86	5.80	5.77	5.75	5.72	5.69	5.66	5.63
5	6.61	5.79	5.41	5.19	5.05	4.95	4.88	4.82	4.77	4.74	4.68	4.62	4.56	4.53	4.50	4.46	4.43	4.40	4.36
6	5.99	5.14	4.76	4.53	4.39	4.28	4.21	4.15	4.10	4.06	4.00	3.94	3.87	3.84	3.81	3.77	3.74	3.70	3.67
7	5.59	4.74	4.35	4.12	3.97	3.87	3.79	3.73	3.68	3.64	3.57	3.51	3.44	3.41	3.38	3.34	3.30	3.27	3.23
8	5.32	4.46	4.07	3.84	3.69	3.58	3.50	3.44	3.39	3.35	3.28	3.22	3.15	3.12	3.08	3.04	3.01	2.97	2.93
9	5.12	4.26	3.86	3.63	3.48	3.37	3.29	3.23	3.18	3.14	3.07	3.01	2.94	2.90	2.86	2.83	2.79	2.75	2.71
10	4.96	4.10	3.71	3.48	3.33	3.22	3.14	3.07	3.02	2.98	2.91	2.85	2.77	2.74	2.70	2.66	2.62	2.58	2.54
11	4.84	3.98	3.59	3.36	3.20	3.09	3.01	2.95	2.90	2.85	2.79	2.72	2.65	2.61	2.57	2.53	2.49	2.45	2.40
12	4.75	3.89	3.49	3.26	3.11	3.00	2.91	2.85	2.80	2.75	2.69	2.62	2.54	2.51	2.47	2.43	2.38	2.34	2.30
13	4.67	3.81	3.41	3.18	3.03	2.92	2.83	2.77	2.71	2.67	2.60	2.53	2.46	2.42	2.38	2.34	2.30	2.25	2.21
14	4.60	3.74	3.34	3.11	2.96	2.85	2.76	2.70	2.65	2.60	2.53	2.46	2.39	2.35	2.31	2.27	2.22	2.18	2.13
15	4.54	3.68	3.29	3.06	2.90	2.79	2.71	2.64	2.59	2.54	2.48	2.40	2.33	2.29	2.25	2.20	2.16	2.11	2.07
16	4.49	3.63	3.24	3.01	2.85	2.74	2.66	2.59	2.54	2.49	2.42	2.35	2.28	2.24	2.19	2.15	2.11	2.06	2.01
17	4.45	3.59	3.20	2.96	2.81	2.70	2.61	2.55	2.49	2.45	2.38	2.31	2.23	2.19	2.15	2.10	2.06	2.01	1.96
18	4.41	3.55	3.16	2.93	2.77	2.66	2.58	2.51	2.46	2.41	2.34	2.27	2.19	2.15	2.11	2.06	2.02	1.97	1.92
19	4.38	3.52	3.13	2.90	2.74	2.63	2.54	2.48	2.42	2.38	2.31	2.23	2.16	2.11	2.07	2.03	1.98	1.93	1.88
20	4.35	3.49	3.10	2.87	2.71	2.60	2.51	2.45	2.39	2.35	2.28	2.20	2.12	2.08	2.04	1.99	1.95	1.90	1.84
21	4.32	3.47	3.07	2.84	2.68	2.57	2.49	2.42	2.37	2.32	2.25	2.18	2.10	2.05	2.01	1.96	1.92	1.87	1.81
22	4.30	3.44	3.05	2.82	2.66	2.55	2.46	2.40	2.34	2.30	2.23	2.15	2.07	2.03	1.98	1.94	1.89	1.84	1.78
23	4.28	3.42	3.03	2.80	2.64	2.53	2.44	2.37	2.32	2.27	2.20	2.13	2.05	2.01	1.96	1.91	1.86	1.81	1.76
24	4.26	3.40	3.01	2.78	2.62	2.51	2.42	2.36	2.30	2.25	2.18	2.11	2.03	1.98	1.94	1.89	1.84	1.79	1.73
25	4.24	3.39	2.99	2.76	2.60	2.49	2.40	2.34	2.28	2.24	2.16	2.09	2.01	1.96	1.92	1.87	1.82	1.77	1.71
26	4.23	3.37	2.98	2.74	2.59	2.47	2.39	2.32	2.27	2.22	2.15	2.07	1.99	1.95	1.90	1.85	1.80	1.75	1.69
27	4.21	3.35	2.96	2.73	2.57	2.46	2.37	2.31	2.25	2.20	2.13	2.06	1.97	1.93	1.88	1.84	1.79	1.73	1.67
28	4.20	3.34	2.95	2.71	2.56	2.45	2.36	2.29	2.24	2.19	2.12	2.04	1.96	1.91	1.87	1.82	1.77	1.71	1.65
29	4.18	3.33	2.93	2.70	2.55	2.43	2.35	2.28	2.22	2.18	2.10	2.03	1.94	1.90	1.85	1.81	1.75	1.70	1.64
30	4.17	3.32	2.92	2.69	2.53	2.42	2.33	2.27	2.21	2.16	2.09	2.01	1.93	1.89	1.84	1.79	1.74	1.68	1.62
40	4.08	3.23	2.84	2.61	2.45	2.34	2.25	2.18	2.12	2.08	2.00	1.92	1.84	1.79	1.74	1.69	1.64	1.58	1.51
60	4.00	3.15	2.76	2.53	2.37	2.25	2.17	2.10	2.04	1.99	1.92	1.84	1.75	1.70	1.65	1.59	1.53	1.47	1.39
120	3.92	3.07	2.68	2.45	2.29	2.17	2.09	2.02	1.96	1.91	1.83	1.75	1.66	1.61	1.55	1.50	1.43	1.35	1.25
inf	3.84	3.00	2.60	2.37	2.21	2.10	2.01	1.94	1.88	1.83	1.75	1.67	1.57	1.52	1.46	1.39	1.32	1.22	1.00