Tools for analysing designed multiresponse experiments

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In industrial and scientific experimentation multiple and highly correlated responses are common (multi-channel instruments). In such cases it is useful to combine design-of-experiments methodology and multivariate techniques. In this area new methodology has been developed at MATFORSK and a related windows program has been made available (www.matforsk.no/ola/program.htm). This presentation aims to illustrate an approach for analysing multiresponse experiments and the new software will be demonstrated. The design variables can be continuous and/or categorical and the design needs not be perfectly balanced. In the univariate special case some modifications of the standard general-linear-models analysis are recommended. Proper Type II Sums of Squares (SS) are more efficient and reliable than Type III SS. Instead of reporting the SS's directly they are divided by the total SS to obtain a sort of explained variance measure. Instead of focusing on parameter estimates, the significant effect will be illustrated by different (adjusted) mean values and predictions at various level combinations. In the multivariate case the explained variance measure is based on the univariate SS's summed over all responses. Significance tests are performed using the new tools, 50-50 MANOVA and rotation testing (adjusted p-values). Multivariate mean values and predictions can be illustrated in a principal component score plot or directly as curves. In this talk, the demonstration and discussion will be based on examples from production of cheese and fishmeat loaves with multiple responses from spectroscopy, rheology and sensory evaluation. Analysis of data generated by the process simulation game from Greenfield Research will also be included.

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Windows program for 50-50 MANOVA

- This presentation is mainly an interactive demonstration of this homemade windows program.
- Available at http://www.matforsk.no/ola/program.htm
- Features:
  - New method for multivariate ANOVA/GLM
  - Illustration of effects
    - (adjusted) mean curves
    - in a principal component score plot
  - Adjusted p-values by rotation testing (new method)

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Production of fishmeat loaves

runOrder	Day	Fish%	PriceCat	MilkProt	Hardness
17	2	35.0	1	5	3.78048
9	1	35.0	2	6	3.84826
18	2	35.0	3	7	3.94864
7	1	37.5	1	4	3.72921
16	2	37.5	2	5	3.88381
8	1	37.5	3	6	3.94078
14	2	40.0	1	3	3.75849
6	1	40.0	2	4	3.79866
15	2	40.0	3	5	3.95267
4	1	42.5	1	2	3.70348
13	2	42.5	2	3	3.66002
5	1	42.5	3	4	3.83951
11	2	45.0	1	1	3.73655
3	1	45.0	2	2	3.83846
12	2	45.0	3	3	3.84729
1	1	47.5	1	0	3.71353
10	2	47.5	2	1	3.69649
2	1	47.5	3	2	3.79089

- Fish% and PriceCat: Balanced design
- Fish% and MilkProt: Unbalanced design
- Multiple responses from sensory evaluation

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Hardness as response

Least Squares Means for Hardness

PriceCat	Mean	SE Mean
1	3.737	0.01876
2	3.788	0.01876
3	3.887	0.01876
Fish%		
35.0	3.862	0.02680
37.5	3.849	0.02680
40.0	3.839	0.02680
42.5	3.732	0.02680
45.0	3.810	0.02680
47.5	3.731	0.02680

----- 50-50 MANOVA VERSION 1.5exe ----- 1 responses:

Source	DF	exVarSS	nPC	nBu	exVarPC	exVarBU	p-Value
Day	1	0.006774	1	0	1.000	1.000	0.522500
Fish%	5	0.356549	1	0	1.000	1.000	0.022353
PriceCat	2	0.504209	1	0	1.000	1.000	0.000981
Error	9	0.137710 - STANDARDIZATION ON ----------					

----- 50-50 MANOVA VERSION 1.5exe ----- 1 responses:

Source	DF	exVarSS	nPC	nBu	exVarPC	exVarBU	p-Value
Day	1	0.000060	1	0	1.000	1.000	0.958269
Fish%	1	0.228991	1	0	1.000	1.000	0.007031
PriceCat	1	0.487258	1	0	1.000	1.000	0.000537
Fish%*PriceCat	1	0.034368	1	0	1.000	1.000	0.226919
Fish%*Fish%	1	0.000118	1	0	1.000	1.000	0.941576
PriceCat*PriceCat	1	0.016951	1	0	1.000	1.000	0.387976
Error	11	0.230782 - STANDARDIZATION ON ----------					

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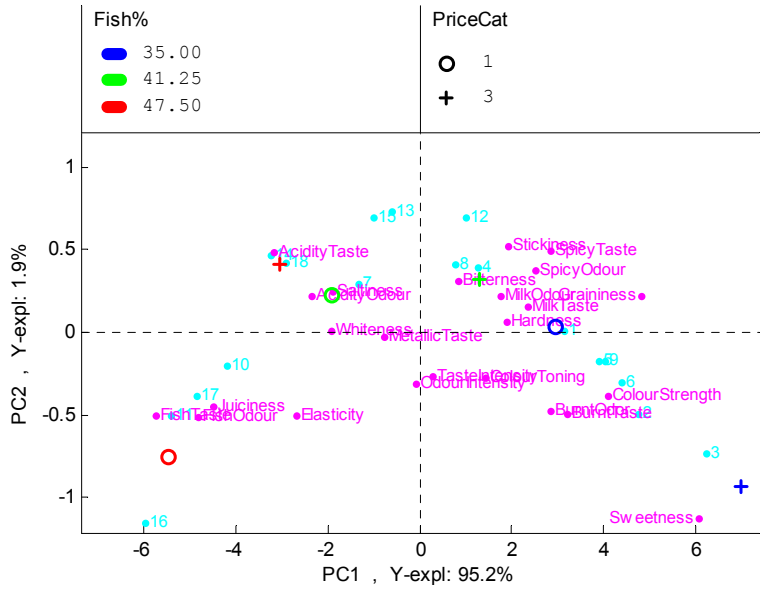
Sensory responses

```
-----  50-50 MANOVA  VERSION 1.5exe -----  24 responses:
  Source              DF        exVarSS nPC nBu exVarPC exVarBU    p-Value
  Day                  1       0.004024   2   3   0.901   0.966   0.426353
  Fish%                1       0.666058   1   4   0.966   0.993   0.000011
  PriceCat             1       0.122146   1   4   0.909   0.978   0.003748
  Fish%*PriceCat       1       0.009665   2   3   0.900   0.966   0.009904
  Fish%*Fish%          1       0.010082   2   3   0.894   0.965   0.004787
  Error               12       0.175275 - STANDARDIZATION OFF ------------
```

Production of cheese

Block	A	B	C	D	Yield
1	3.150	2.20	7.0	36.50	54.4
1	3.500	2.20	7.0	39.00	58.3
1	3.500	1.70	0.0	39.00	57.5
1	3.150	1.70	7.0	39.00	56.9
1	3.500	2.20	0.0	36.50	55.8
1	3.150	2.20	0.0	39.00	57.5
2	3.325	1.95	3.5	37.75	56.4
2	3.150	1.70	7.0	39.00	57.2
2	3.500	2.20	0.0	36.50	56.0
2	3.325	1.95	3.5	37.75	56.9
2	3.150	1.70	0.0	36.50	55.5
2	3.500	2.20	7.0	39.00	58.2
2	3.325	1.95	3.5	37.75	56.5
2	3.500	1.70	0.0	39.00	58.2
2	3.500	1.70	7.0	36.50	55.6
2	3.325	1.95	3.5	37.75	56.7
2	3.150	2.20	0.0	39.00	56.9
3	3.500	1.95	0.0	37.30	56.1
3	3.150	1.95	0.0	38.20	56.5
3	3.500	1.95	0.0	37.30	56.6
3	3.500	1.95	0.0	37.30	57.3
3	3.150	1.95	0.0	38.20	56.8
3	3.500	1.95	0.0	37.30	57.0
3	3.150	1.95	0.0	38.20	57.6

- Partly replicated fractional design
- + centre points
- + extra points

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IR spectra as multiple responses

```
-----  50-50 MANOVA  VERSION 1.5exe -----  477 responses:
  Source    DF        exVarSS nPC nBu exVarPC exVarBU    p-Value
  Block      2       0.229754   2   6  0.751   0.981    0.000004
  A          1       0.059568   2   6  0.737   0.977    0.058142
  B          1       0.041292   2   6  0.724   0.977    0.084017
  C          1       0.038253   2   6  0.717   0.976    0.098135
  D          1       0.315012   2   6  0.817   0.985    0.000052
  Error     17       0.366951 - STANDARDIZATION OFF ------------


-----  50-50 MANOVA  VERSION 1.5exe -----  477 responses:
  Source    DF        exVarSS nPC nBu exVarPC exVarBU    p-Value
  Block      2       0.192720   2   4  0.775   0.972    0.000000
  A          1       0.053407   2   4  0.825   0.965    0.064514
  B          1       0.037455   2   4  0.803   0.965    0.060738
  C          1       0.035440   2   4  0.791   0.965    0.118843
  D          1       0.315012   2   4  0.883   0.980    0.000001
  A*D        1       0.023918   2   4  0.781   0.963    0.401477
  B*D        1       0.045719   2   4  0.748   0.963    0.006130
  C*D        1       0.012780   2   4  0.808   0.963    0.700330
  D*D        1       0.009110   2   4  0.792   0.957    0.903666
  Error     13       0.274129 - STANDARDIZATION OFF ------------
```

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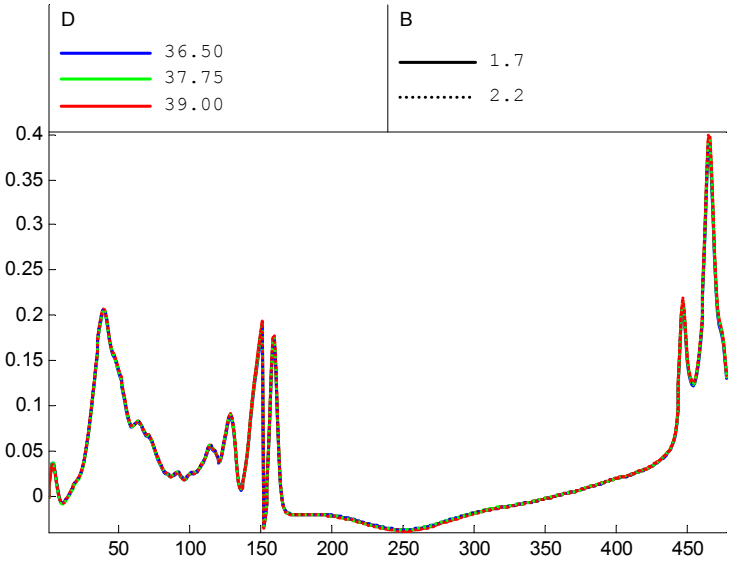
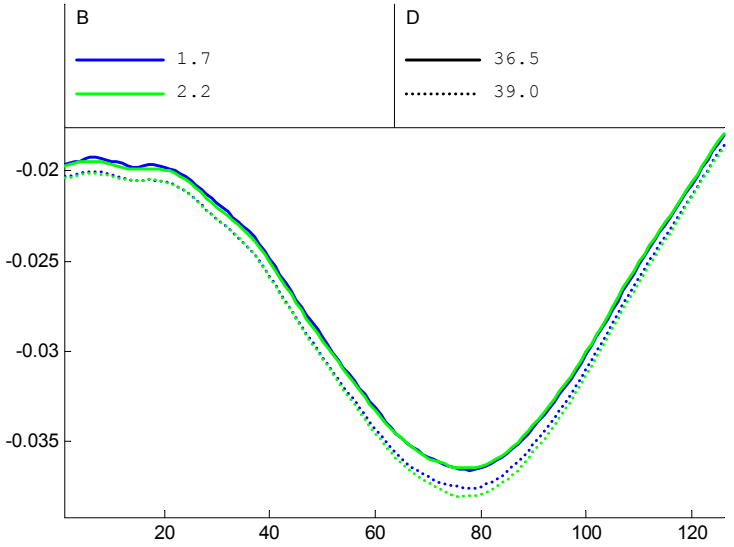
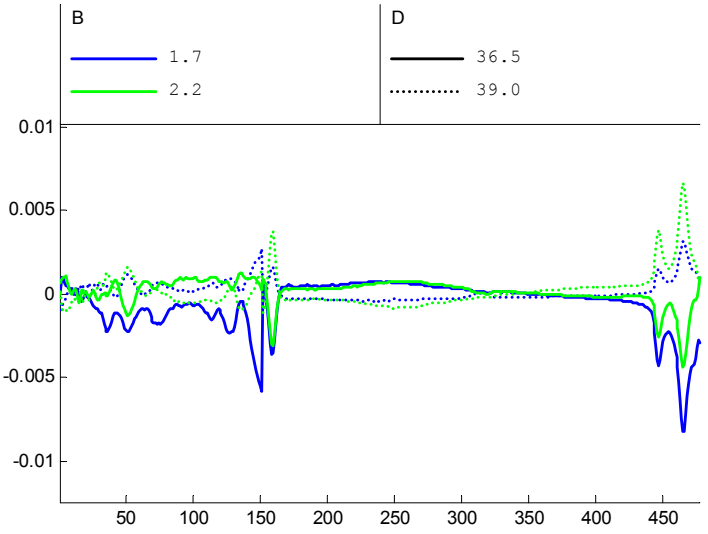
All wavelengths



Some wavelengths



Mean centred spectra



B*D: Adjusted p-values by rotation testing

rankNr	varNr	varName	pRaw	p999999
1	147	y147	0.000024	0.001778
2	151	y151	0.000026	0.001950
3	148	y148	0.000027	0.002000
4	150	y150	0.000032	0.002282
5	149	y149	0.000040	0.002823
6	146	y146	0.000041	0.002854
7	145	y145	0.000091	0.005635
8	125	y125	0.000100	0.006085
9	144	y144	0.000139	0.007935
10	126	y126	0.000158	0.008858
11	75	y75	0.000277	0.014239
12	124	y124	0.000285	0.014579
13	76	y76	0.000299	0.015183
14	74	y74	0.000459	0.021667
15	143	y143	0.000485	0.022615
16	73	y73	0.000607	0.027043
17	77	y77	0.000764	0.032429
18	127	y127	0.000841	0.035041
19	72	y72	0.001175	0.045755
20	78	y78	0.001669	0.060396

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Univariate special case

- General linear model (continuous and categorical)
- Type II Instead of Type III Sums of Squares
  - Unlike SAS Type II also for continuous variables
  - More powerful and scaling problems are avoided
- Illustrating effects of categorical variables
  - Least Squares Means (by using SAS's OM-option)
- Illustrating effects of continuous variabls
  - (Mean)-predictions at min and max
  - and mid point when second order
- Report sums of squares as the fraction of the total sums of squares (explained variance)

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Multiple responses

- Significance testing
  - 50-50 MANOVA
  - Adjusted p-values by rotation testing
- Illustration of effects
  - (adjusted) mean curves
  - in a principal component score plot
- Explained variance based on sum of sums of squares

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