TMA4267 Linear statistical models

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Today and next time

Three scientific publications (2004, 2005, 2012) illustrating the use of 2-level factorial experiments, and motivating the theory that we cover in TMA4267

Example 1

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Process Biochemistry 40 (2005) 779–788

PROCESS BIOCHEMISTRY

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Biosorption of chromium using factorial experimental design

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2^3 full factorial design, duplicated

Wikipedia:
Biosorption can be defined as the ability of biological materials to accumulate heavy metals from wastewater through metabolically mediated or physico-chemical pathways of uptake.[2] Though using biomass in environmental cleanup has been in practice for a while, scientists and engineers are hoping this phenomenon will provide an economical alternative for removing toxic heavy metals from industrial wastewater and aid in environmental remediation.

Example 1: Biosorption of chromium using factorial experimental design

- Aim: Removal of Cr^{3+} (and Cr^{6+})
- Design: 2^3 factorial design
- Factors:
  - *T*: temperature (29 and 55 degrees celcius)
  - *C*: metal concentration (10 and 1200 mg/L)
  - *pH*: pH (2.0 and 6.0)
- Response: Efficiency of chromium removal after 6h exposition time

Example 1: Biosorption of chromium using factorial experimental design

(Intercept)	Tmp	Conc	pH	Tmp:Conc	Tmp:pH	Conc:pH	Tmp:Conc:pH
1	1	1	1	1	1	1	1
1	1	1	-1	1	-1	-1	-1
1	1	-1	1	-1	1	-1	-1
1	1	-1	-1	-1	-1	1	1
1	-1	1	1	-1	-1	1	-1
1	-1	1	-1	-1	1	-1	1
1	-1	-1	1	1	-1	-1	1
1	-1	-1	-1	1	1	1	-1

Example 1: Biosorption of chromium using factorial experimental design

Table 2
Experimental factorial design results for Cr^{3+}

Factor			Species		
T	C	pH	Cr^{3+}		
			Removal efficiency (%)[a]		Average (%)
1	1	1	75.2	74.8	75.0
1	1	−1	11.4	5.4	8.4
1	−1	1	62.7	56.4	59.6
1	−1	−1	82.9	83.5	83.2
−1	1	1	99.5	99.5	99.5
−1	1	−1	2.5	17.3	9.9
−1	−1	1	62.3	68.9	65.6
−1	−1	−1	73.4	74.2	73.8

[a] Experiments in duplicate.

Main and interaction effects

From the note Design of experiments, J. Tyssedal

Definition of main effect:

For two-level designs we define the main effect of a factor as: Expected average response when the factor is on the high level – expected average response when the factor is at the low level.

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Definition

The interaction between two factors is defined as: Half the main effect of a factor when the other is on the high level – half the main effect of a factor when the other factor is at its low level.

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−1	−1	−1	73.4	74.2	73.8

[a] Experiments in duplicate.

Example 1: Biosorption of chromium using factorial experimental design

Table 3
Statistical parameters for 2^3 design

Factor	Species		
	Cr^{3+}		
	Coefficient	Standard error	Effect
Average	59.4	1.15	59.4
T	−2.8	1.15	−5.6
C	−11.2	1.15	−22.3
pH	15.5	1.15	31.1
TC	−3.7	1.15	−7.3
*T*pH	−4.8	1.15	−9.6
*C*pH	23.5	1.15	47.0
*TC*pH	−0.94	1.15	−1.9

Example 1: Biosorption of chromium using factorial experimental design

Table 4
Analysis of variance — full model fitting for Cr^{3+}

Factor	Statistics				
	Sum of squares	Degrees of freedom	Mean square (MS)	F_o	*P*-value
T	128.26	1	128.26	6.0	0.039397
C	1,995.86	1	1,995.86	94.1	0.000011
pH	3,865.73	1	3,865.73	182.2	0.000001
TC	215.36	1	215.36	10.1	0.012880
*T*pH	369.60	1	369.60	17.4	0.003106
*C*pH	8,840.70	1	8,840.70	416.7	0.000000
*TC*pH	14.25	1	14.25	0.7	0.436193
Error	169.73	8	21.22		
Total	15,599.47	15			

$F_o = MS_{FACTOR}/MS_{ERROR}$; $R^2 = 0.9891$; R^2 adj. $= 0.9796$.

Example 1: Biosorption of chromium using factorial experimental design

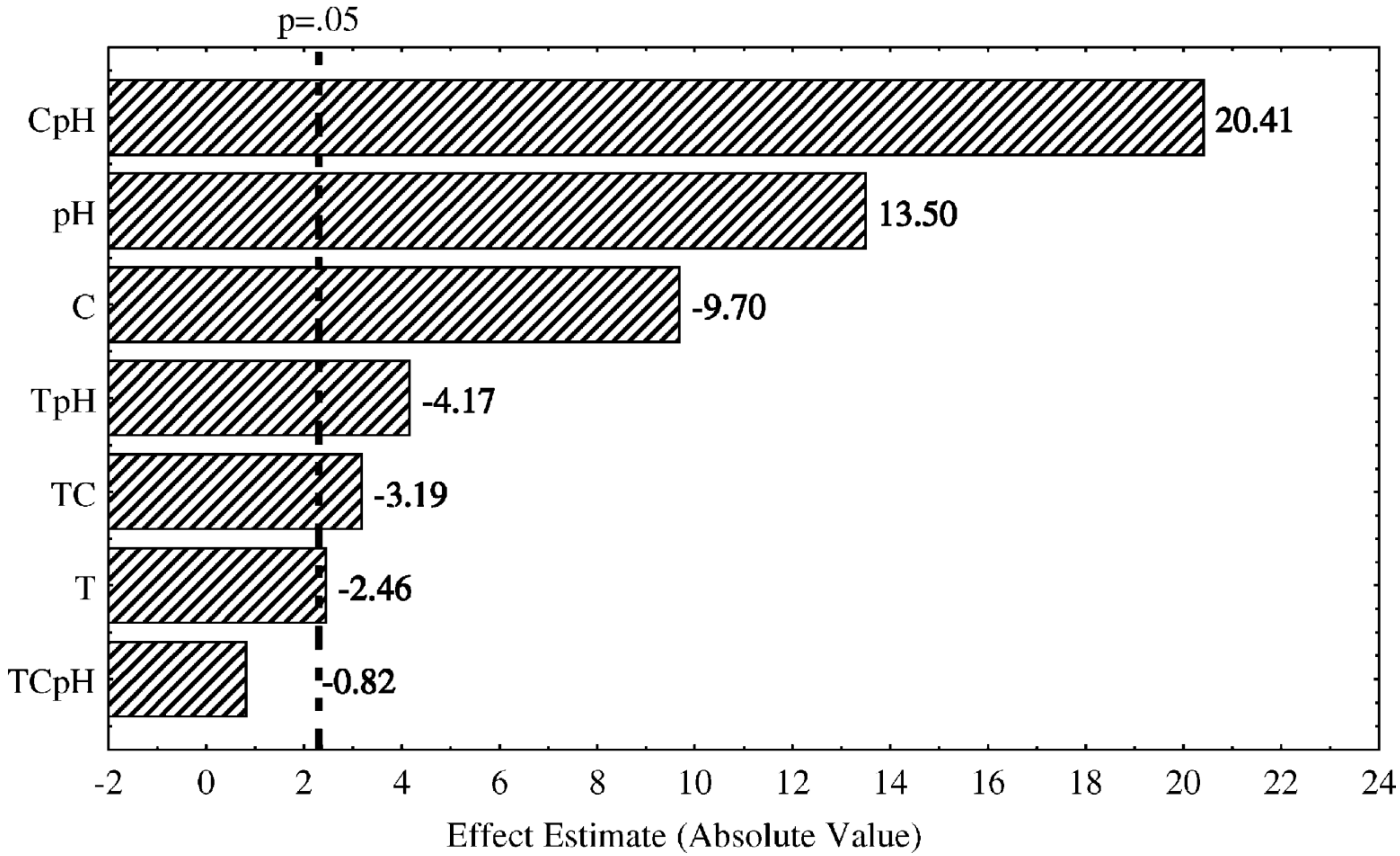

Fig. 1. Pareto chart of effects on the removal efficiency of Cr^{3+}.

Example 2

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Journal of Hazardous Materials B135 (2006) 165–170

Journal of Hazardous Materials

www.elsevier.com/locate/jhazmat

Phosphate removal from water by fly ash: Factorial experimental design

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2^3 full factorial design

Example 2: Phosphate removal from water by fly ash: Factorial experimental design

Table 1
Values of operating variables used in the designed set of experiments

Operating variable	−1	1
x_1 (phosphate concentration) ($mg\,l^{-1}$)	25	50
x_2 (fly ash dosage) ($g\,l^{-1}$)	0.5	2
x_3 (pH_0)	2.9	5.5

Table 3
Experimental results of 2^3 designs for the % E

Experiments	x_1	x_2	x_3	Y_1
1	−1	−1	−1	17.16
2	1	−1	−1	1.5
3	−1	1	−1	99.41
4	1	1	−1	41.22
5	−1	−1	1	26.4
6	1	−1	1	1.1
7	−1	1	1	99.6
8	1	1	1	49.56

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x_3 (pH_0)	2.9	5.5

Table 4
Results of regression analyzing for % E (Y_1)

	Coefficient	S.E.	*t*-value
Intercept	41.99375	0.134519	–
x_1	−18.6488	0.134519	−138.633
x_2	30.45375	0.134519	226.3903
x_3	2.17125	0.134519	16.14086
x_1x_2	−8.40875	0.134519	−62.5098
$x_1x_2x_3$	2.22375	0.134519	16.53114

Example 3: Computational run time

Recall our 2^2 experiment:

y: computation run time of algorithm that
samles m poisson variables and returns an average

A: for loop or built-in Poisson(m)

B: sum/length or built-in mean

Design:

	A	B	AB
1	-1	-1	1
1	-1	1	-1
1	1	-1	-1
1	1	1	1

Problem: We have to use two different computers (for some reason...)

Blocking in 2^3: using example 1

2 blocking factors: try TCpH and CpH

TCpH = 1, CpH = 1

TCpH = -1, CpH = 1

TCpH = 1, CpH = -1

TCpH = -1, CpH = -1

Tmp	Conc	pH	Tmp:Conc	Tmp:pH	Conc:pH	Tmp:Conc:pH
1	1	1	1	1	1	1
1	1	-1	1	-1	-1	-1
1	-1	1	-1	1	-1	-1
1	-1	-1	-1	-1	1	1
-1	1	1	-1	-1	1	-1
-1	1	-1	-1	1	-1	1
-1	-1	1	1	-1	-1	1
-1	-1	-1	1	1	1	-1

Note: first column (T) equal in all blocks! Now temperature is also confounded...

Blocking in 2^3: using example 1

2 blocking factors: try TC and TpH

Tmp	Conc	pH	Tmp:Conc	Tmp:pH	Conc:pH	Tmp:Conc:pH
1	1	1	1	1	1	1
1	1	-1	1	-1	-1	-1
1	-1	1	-1	1	-1	-1
1	-1	-1	-1	-1	1	1
-1	1	1	-1	-1	1	-1
-1	1	-1	-1	1	-1	1
-1	-1	1	1	-1	-1	1
-1	-1	-1	1	1	1	-1

Note: none of the main effects are confounded

Note: all two-factor interactions are confounded