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Two-level Factorial Experiment for Measurement of Cd on Equipment AA Analyst

David M. Harutyunyan

Center for Ecological Noosphere Studies of NAS of RA
e-mail: harutyunyan_david@yahoo.com

Abstract

The results of various methods in analytical chemistry are subject to different factors of countable number. Some of them may have insignificant, others significant impact on the results of analysis, which will orient the specialists to make true analysis to the extent of permissibility by holding their magnitudes at the optimal levels.

1. Introduction

In many applications we are interested in investigation of influence of several factors on a response variable [2]. Here we carry out a sequence of experiments in which we observe the yield of the process under different *atomization temperature* and different levels of *process time*. The yield is assumed to be measurement of cadmium concentration by AA Analyst. Operator familiar with the process certainly told us about the feasible ranges for atomization temperature and process time. In this example we selected two levels of temperature T: a low level of 1300 degrees (-) and a high level of 1400 degrees (+). We also selected two levels for process time P: a low level of 2 seconds (-) and a high level of 3 second (+). We use "-" and "+" codes to abbreviate the low and high values.

2. Factorial experiment in two factors

We carry out a simple *factorial experiment*. In a factorial experiment one investigates all possible factor-level combinations. Since each of two factors is studied at two levels, there is a total of four factor-level combinations. These combinations (in the original factor levels, as well as in coded units "+" and "-" for high and low levels) are listed in Table 1. We carried out eight runs as we replicated the experiment once, and we randomized the order of eight runs. The yields of the two runs at each of the four factor-level combinations, as well as their average, are listed in Table 2 [3].

Table 1

		Yield (in ug/ml)		
Temperature	Time	Average	Run1	Run2
1300 degrees	2 seconds	0.006	0.012	0.000
1400 degrees	2 seconds	0.06	0.100	0.020
1300 degrees	3 seconds	0.168	0.120	0.215
1400 degrees	3 seconds	0.218	0.220	0.215

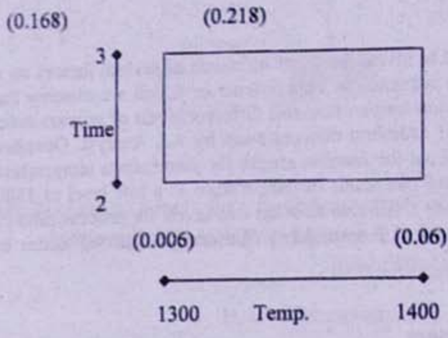
Replicated 2^2 factorial experiment

Table 1

		Yield (in ug/ml)		
Temperature	Time	Average	Run1	Run2
-	-	0.006	0.012	0.000
+	-	0.06	0.100	0.020
-	+	0.168	0.120	0.215
+	+	0.218	0.220	0.215

Replicated 2^2 factorial experiment

Average yields are listed first. Yields of replicates are shown in Run1 and Run2 columns



We create a table; in the first column (for the first factor) we enter the sequence: "- + - +". The column starts with a "-" sign, and the signs alternate each time. The second column (for the second factor) is written as "- - + +". It starts with 2 minus signs, "- -", and signs alternate in groups of two. The rows of this table give us the levels of the four runs. The first one is the one where both factors are at their low levels; the second run is the one where the first factor is at its high level and the second factor is at its low level; and so on. This arrangement of four runs is called *standard order* and t is useful as it gives us a simple rule for writing sown all possible factor-level combinations.

Geometrically, the four factor-level combinations represent the corners of the square in Table 2.

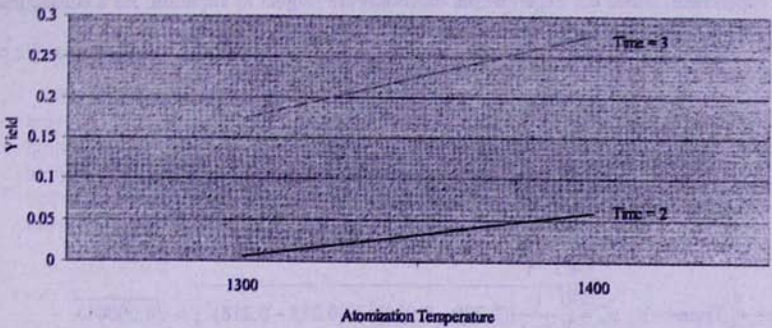
3. Analysis of data from two-level factorial design

The average yields at the four factor-level combinations of the 2^2 factorial experiment are used to estimate the effects of the two factors on the response [2].

The average yields, depicted at the four corners of the square in Table 2, are used to estimate the effects of temperature and process time. Figure 1 expresses the same information graphically. There we plot yields for two levels of atomization temperature, separately for each level of process time; observations that come from the same process time are connected.

The effect of a 100 degrees change in temperature from 1300 degrees (-) to 1400 (+) is estimated by the difference of the yield averages at temperature 1400 and 1300. The yields at temperature 1400 degrees are 0.06 and 0.218, and those at 1300 degrees are 0.006 and 0.168.

Figure 1



Graphical display of the results of the 2^2 factorial experiment

Thus, the estimated effect T of temperature is

$$T=\frac{0.06+0.218}{2}-\frac{0.006+0.168}{2}=0.139-0.087=0.052$$

The estimated effect T=0.052 implies that a 100-degree temperature change from 1300 to 1400 degrees increases the yield by 0.052 ug/ml.

Similarly, the effect of P of a process time change from 2 (-) seconds to 3 (+) seconds is estimated as the difference of the yield averages at 3 (+) and 2 (-) seconds:

$$P=\frac{0.168+0.218}{2}-\frac{0.006+0.06}{2}=0.193-0.033=0.16$$

The result, P = 0.16, implies that an increase in the process time from 2 to 3 seconds decreases the yield by 0.16 ug/ml. These effects are called the *main effects* [1,3].

In many cases it happens that the effect of a change in one factor depends on the level of the other factor(s); in particular case the temperature effect may change dependent on the level of process time. It could be that the impact of a temperature change at a process time of 2 seconds is very different from the impact of a temperature change at a temperature change at a process time of 3 seconds.

We can check whether this is the case. Presence or absence of an interaction between the factors temperature and process time can be seen from figure 1. In this graph the two yield lines, for low and high levels of P, are almost parallel. This means that the temperature effects at two levels of P are pretty much the same.

The *interaction* between the factors, T×P is quantified as one half of the difference of the main effect of temperature at process time of 3 seconds (+) and the main effect of temperature at process time of 2 seconds (-).

T×P = [(0.218-0.168)-(0.06-0.006)]/2 = -0.004

Our data are too small. Usually if this coefficient is 0 or small in absolute value, then we say that there is no interaction between the two factors. The presence of an interaction negatively influences interpretation of main effects. Figure 1 is also called the interaction plot where the parallel lines serve the evidence for no (or little) interaction.

4. Determination of the statistical significance of estimated effects

The outcomes of the experiments are affected by factors other than those that are controlled in the experiment; hence the experimental outcomes are subject to variation. As a consequence the estimated effects are subject to sampling variability.

We use two experiments, carried out ate each of the four factor-level combinations. We can use these two observations to calculate the standard deviation, that are given by

(Temp= -; Time= -): $s_1 = \sqrt{\frac{1}{2-1}[(0.012-0.006)^2 + (0.000-0.006)^2]} = \sqrt{0.000072}$

(Temp= +; Time= -): $s_2 = \sqrt{\frac{1}{2-1}[(0.1-0.06)^2 + (0.02-0.06)^2]} = \sqrt{0.0032}$

(Temp= -; Time= +): $s_3 = \sqrt{\frac{1}{2-1}[(0.12-0.168)^2 + (0.215-0.168)^2]} = \sqrt{0.004513}$

(Temp= +; Time= +): $s_4 = \sqrt{\frac{1}{2-1}[(0.220-0.218)^2 + (0.215-0.218)^2]} = \sqrt{0.000013}$

This yields the pooled estimate

$s_{pooled} = \sqrt{(0.000072 + 0.0032 + 0.004513 + 0.000013)/4} = \sqrt{0.016726/4} = 0.044$

and the standard error of each estimated effect

$StdDev(effect) = (0.044)\sqrt{\frac{1}{(2)2^{2-2}}} = 0.031$

Approximate 95% confidence intervals for the effects are obtained by adding and subtracting (2)(0.031)=0.062 from the estimates. The T×P interaction effect (which was -0.004) is not statistically significant. This is because the interval -0.004±0.062, or (-0.066, 0.058), includes 0. Thus there is at most, very minor interaction between atomization temperature and process time. The absence of any appreciable interaction is also evident from the interaction plot in figure 1, the two lines at that graph are almost parallel [1].

Among the main effects (0.052 for temperature and 0.16 for process time) only the process time is larger than two standard errors. Thus there is considerable evidence that this effect is larger than zero. This factor influences the yield of the process.

References

[1] Box, G.E.P., W.G. Hunter, and J.S. Hunter, (1978). Statistics for Experiments. New York: Wiley.

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[3] Montgomery, D.C. (1996) Introduction to Statistical Quality Control, 3rd edition. New York: Wiley.

AA Analyst սարքավորմամբ Կադմիումի չափման երկմակարդակ ֆակտորիալ էքսպերիմենտ

Դ. Մ. Հարությունյան

Ամփոփում

Վերլուծական քիմիայում բազմաթիվ մեթոդների արդյունքներն ենթակա են հաշվելի թվով տարբեր գործոնների ազդեցությունների: Նրանցից մի քանիսը կարող են ունենալ զգալի, մյուսները՝ ոչ զգալի ազդեցություն տարրալուծման արդյունքների վրա, որոնք կկողմնորոշեն մասնագետներին, վերջիններիս մեծությունները օպտիմալ մակարդակներում պահելով, թույլատրելիության սահմաններում ճշմարիտ վերլուծություն կատարելու համար: