



Małgorzata Złotoś 

University of Economics in Katowice, Faculty of Management, Department of Statistics
Econometrics and Mathematics, malgorzata.zlotos@ue.katowice.pl

On the Use of Permutation Tests in the Analysis of the Factorial Design of Experiment Results

Abstract: An experimental design is one of the tools which are used in statistical quality control. The proper implementation of experimental design results in the improvement of technological outcomes of a manufacturing process, which in turn leads to the enhancement of economic results. Permutation tests, among other things, form a group of resampling methods which are used to verify statistical hypotheses. These tests, unlike parametric ones, do not entail the fulfilment of strict criteria and may be used for a small number of observations. The presented article deals with the use of permutation tests in the design of experiments. The proposed method will be presented with reference to selected empirical data.

Keywords: Tukey's test, Fisher Least Significant Difference Method, design of experiments, permutation tests

JEL: C99, C12, C15

1. Introduction

The first application of experimental design methods concerning agricultural experiments was carried out by R. A. Fisher (Kończak, 2007; Wawrzynek, 2009). Intensive development of design of experiments methods in production processes began in the 1960s. The introduction of the design of experiments in the planning of production processes contributed to a decrease in production costs and to the improvement of technological parameters (Kończak, 2007; Wawrzynek, 2009). Moreover, designs of experiments are used, among others, in biology, medicine and spatial data analysis. Currently, statistical methods are sought that could be an alternative to the classical statistical methods used in design of experiments.

When R. A. Fisher analysed the results of agricultural experiments, he tried to determine the procedure of permutation tests. Intensive development of technology allowed for using permutation methods in many areas of statistical data analysis. The aim of the paper is to present the appropriate use of selected permutation tests in the analysis of experimental results.

2. Factorial designs of experiments

In statistical quality control, methods of designing experiments are usually used to determine factors that most significantly affect the response variable. Moreover, the design of experiments allows us to estimate the values of factors for which the response variable achieves the smallest variability or the proper value.

The proper use of experimental design methods requires adequate preparation which should consist of the following steps (Montgomery, 1997):

- 1) recognise and define the problem by determining all the aspects, circumstances and potential objectives of the experiment;
- 2) appropriately select the factors, their levels and ranges, assess the chances of considering them in the experiment;
- 3) define the response variable;
- 4) choose a proper design of the experiment, i.e. determine the number of experimental trials and the possible randomisation restrictions;
- 5) perform the experiment;
- 6) analyse the results using statistical methods;
- 7) formulate conclusions and recommendations resulting from the analysis of the results.

An experiment is defined as the sequence of n experimental trials. An experimental trial is a single result of the value of response variable Y , with the fixed values of factors X_1, X_2, \dots, X_m . To design an experiment is to determine the combination of the levels of selected factors in subsequent experiments. The dependence

of response variable Y on the values of factors is described as a mathematical model and it can be defined in particular as a general linear model (Wawrzynek, 1993).

Among the designs of experiments used in practice, factorial designs of experiments should be distinguished. First of all, it is possible to consider the design of an experiment which takes into account one factor A at a levels, i.e. the single-factor experiment (Kończak, 2007). The single-factor experiment is presented in Table 1.

Table 1. The single-factor experiment

Levels of factor A	Values of response variable				y_i	\bar{y}_i
	1	2	...	k		
1	y_{11}	y_{12}	...	y_{1k}	$y_{1.} = \sum_{j=1}^k y_{1j}$	$\bar{y}_{1.} = \frac{1}{k} y_{1.}$
2	y_{21}	y_{22}	...	y_{2k}	$y_{2.} = \sum_{j=1}^k y_{2j}$	$\bar{y}_{2.} = \frac{1}{k} y_{2.}$
...
a	y_{a1}	y_{a2}	...	y_{ak}	$y_{a.} = \sum_{j=1}^k y_{aj}$	$\bar{y}_{a.} = \frac{1}{k} y_{a.}$

Source: own elaboration

The dependence between the factor A and the response variable Y can be presented by means of the following model:

$$y_{ij} = \mu + \tau_i + \varepsilon_{ij}, \tag{1}$$

where

y_{ij} – the value of j -th observation of the response variable for the level i of factor A ,
 μ – the mean of the response variable Y ,

τ_i – the deviation of mean value of the variable Y when the factor A is at the level i ,

ε_{ij} – random error of the j -th observation of the response variable for the level i of factor A . It is assumed that the errors are independent and $\varepsilon_{ij} \sim N(0, \sigma^2)$.

On the basis of analysis of variance of experimental results, it is possible to determine whether the change of factor (A) levels has an influence on the value of response variable Y (Elandt, 1964; Montgomery, 1997).

The number of experimental factors taken into consideration may be determined individually. Moreover, it is possible that the factors occur at a different number of levels (Montgomery, 1997; Ryan, 2007; Lawson, 2015). If this is the case, what is considered is the design of an experiment in which:

- 1) m_1 factors occur at p_1 levels
- 2) m_2 factors occur at p_2 levels

3) ...

4) m_k factors occur at p_k levels,

where $m_1 + m_2 + \dots + m_k = m$. The design of an experiment consists of $p_1^{m_1} \cdot p_2^{m_2} \cdot \dots \cdot p_k^{m_k}$ experimental trials and may be used to estimate the determined response surface function (Wawrzynek, 2009). Table 2 presents the design of an experiment which takes into account two factors occurring at p_1 and p_2 levels and k replications of the experiment.

Table 2. The design of an experiment for two factors occurring at a different number of levels.

No.	X_1	X_2	Values of response variable				y_i	\bar{y}_i
			1	2	...	k		
1	$x_1^{(1)}$	$x_1^{(2)}$	y_{11}	y_{12}	...	y_{1k}	$y_{1.} = \sum_{j=1}^k y_{1j}$	$\bar{y}_{1.} = \frac{1}{k} y_{1.}$
2	$x_1^{(1)}$	$x_2^{(2)}$	y_{21}	y_{22}	...	y_{2k}	$y_{2.} = \sum_{j=1}^k y_{2j}$	$\bar{y}_{2.} = \frac{1}{k} y_{2.}$
3	$x_1^{(1)}$	$x_3^{(2)}$	y_{31}	y_{32}	...	y_{3k}	$y_{3.} = \sum_{j=1}^k y_{3j}$	$\bar{y}_{3.} = \frac{1}{k} y_{3.}$
...	
n	$x_{p_1}^{(1)}$	$x_{p_2}^{(2)}$	y_{n1}	y_{n2}	...	y_{nk}	$y_{n.} = \sum_{j=1}^k y_{nj}$	$\bar{y}_{n.} = \frac{1}{k} y_{n.}$

Source: own elaboration

One of the possible analyses of experimental results is to determine if there is any difference between the means of response variable, replication in particular, and, therefore, whether there exist factors influencing the response variable which have not been included in the experiment.

3. Permutation tests

Permutation tests were mentioned for the first time in 1925 in R. A. Fisher's paper titled *Statistical Methods for Research Workers*. Later on, in 1937, more formally, the construction of permutation tests was described by E. J. Pitman. At that time, permutation tests were not widely applied because of calculation difficulties. It was not until the beginning of the 21st century, when the computing power of computers increased significantly, that the intense development of permutation methods took place.

The concept of a permutation test should be understood as a general method for estimating the probability of an event occurring. In the theory of permutation tests, it is possible to define the following three approaches (Berry, Johnston, Mielke Jr, 2014):

- 1) exact permutation test;
- 2) moment approximation permutation test;
- 3) resampling permutation test.

Nowadays, the most popular approach is the resampling test. This type of permutation test leads to the analysis of a subset of all data set permutations. In practice, the number of data permutations should be at least 1,000. The scheme of a permutation test can be defined in the following stages (Good, 2005):

1. Define the null-hypothesis and the alternative hypothesis.
2. Choose the formula of testing statistic T .
3. Count the value of the test statistic T_0 for the sample.
4. Count the value of the test statistic T for N permutations of a data set to obtain the set $\{T_1, T_2, \dots, T_N\}$.
5. Determine the ASL (*achieved significance level*) value and make the appropriate decision.

If a two-sided alternative hypothesis is defined, the value of ASL can be rewritten as follows:

$$ASL = P(|T_i| \geq |T_0|). \quad (2)$$

The approximate value of ASL is calculated using the following formula:

$$A\hat{S}L = \frac{\text{card}\{i: |T_i| \geq |T_0|\}}{N}. \quad (3)$$

If the value of estimated ASL is lower than the significance level, the null hypothesis is rejected. Otherwise, there is no reason why the null hypothesis should be rejected.

In the specialist literature, the difference between parametric tests and permutation tests is defined as follows (Berry, Johnston, Mielke Jr, 2014):

1. Permutation tests use only sample data.
2. The absence of assumptions about the distribution of the response variable.
3. It is possible to consider a sample with a small number of observations.
4. Resistance to the outliers.

4. The comparison of experimental results

If the comparison of many average values is the result of an experiment, the multiple comparison methods should be used. Out of four methods of multiple comparison for average values, Montgomery (2001) favours Tukey's Test and Fisher's Least Significant Difference Method.

Tukey's Test

In order to test the equality of all pairs of treatment means, the hypothesis statements can be written as follows

$$H_0 : \mu_i = \mu_j \quad (4)$$

$$H_1 : \mu_i \neq \mu_j$$

for $i \neq j$. The test statistic is based on the following statistic distribution:

$$q = \frac{\bar{y}_{\max} - \bar{y}_{\min}}{\sqrt{\frac{MS_E}{n}}}, \quad (5)$$

where $MS_E = \frac{\sum_{i=1}^a \sum_{j=1}^n (y_{ij} - \bar{y}_i)^2}{N - a}$, whereas \bar{y}_{\max} and \bar{y}_{\min} are the greatest and smallest values of the sample mean. The distribution of statistic q is known (Montgomery, 2001). The test declares two means to be significantly different when the absolute value of their sample difference is greater than:

$$T_\alpha = q_\alpha(a, f) \sqrt{\frac{MS_E}{n}}, \quad (6)$$

where $q_\alpha(a, f)$ is a quantile of the distribution of statistic q for the significance level α and f degrees of freedom.

Fisher's Least Significant Difference Method

To test hypothesis (4), the value of the least significant difference should be calculated as follows:

$$LSD = t_{\alpha/2, N-a} \sqrt{\frac{2MS_E}{n}}. \quad (7)$$

If the following inequality is true

$$|\bar{y}_i - \bar{y}_j| > LSD \quad (8)$$

then μ_i and μ_j means are different at the significance level α .

The results of experiments are usually characterised by a small number of samples, which stems from high costs of particular experimental trials and technical or physical and chemical conditions of prepared experimental trials. If the null hypothesis about the normal distribution of the response variable is not rejected, it is possible that the distribution is non-normal. Then the assumptions of classical

statistical methods, particularly parametric tests, are not fulfilled, so nonparametric methods should be used. Moreover, Pesarin and Salamaso (2010) suggest in these cases the use of permutation tests. The simulation study concerning the power of parametric, non-parametric and permutation tests which are used for the comparison of means shows that the power of permutation tests is greater than the power of non-parametric tests and close to the power of parametric tests (Kończak, 2016).

An alternative method of means comparison in two populations can be the permutation test. The hypotheses (4) are considered here as it was the case with Tukey’s test and Fisher’s Least Significant Difference Method. The test statistic used in this permutation test is in the form of

$$T = \bar{Y}_1 - \bar{Y}_2 . \tag{9}$$

Considering the two-sided alternative hypothesis, the greatest absolute values of statistic T will confirm the validity of the alternative hypothesis. The estimated ASL value can be rewritten as the form

$$A\hat{S}L = \frac{\text{card}\{i : |T_i| \geq |T_0|\}}{N}, \tag{10}$$

where:

- $A\hat{S}L$ – the estimated value of ASL ,
- T_i – the value of the test statistic (9) for the i -th permutation of a data set,
- T_0 – the value of the test statistic (9) for the sample,
- N – the number of permutations of a data set.

No.	Sample I	Sample II
1	X_{11}	X_{12}
2	X_{21}	X_{22}
...
n	X_{n1}	X_{n2}
Mean	\bar{X}_1	\bar{X}_2
Value of test statistic	T_0	

Figure 1. Original data

Source: own elaboration on the basis on Kończak, 2016

The results of the conducted experiment need to be investigated with the use of statistical methods. When the experiment includes more than one factor and k replications, then it should be considered whether the individual experimental

trials should be included in pairs (Montgomery, 2001). When the analysis of experimental results is a comparison of two different averages, the t test for a paired observation should be used (Montgomery, 2001). In particular, it is possible to consider a permutation test for paired observations (Kończak, 2016). The random selection of the sample in the procedure of this test consists in exchanging observations in individual pairs, while maintaining the order of objects. The forms of the original data and the sample data are presented in Figure 1 and Figure 2.

No.	Number of permutations						
	1		2		...	N	
	Sample I	Sample II	Sample I	Sample II	...	Sample I	Sample II
1	X_{12}	X_{11}	X_{11}	X_{12}	...	X_{11}	X_{12}
2	X_{21}	X_{22}	X_{22}	X_{21}	...	X_{21}	X_{22}
...
n	X_{n1}	X_{n2}	X_{n1}	X_{n2}	...	X_{n2}	X_{n1}
Mean	\bar{X}_{11}	\bar{X}_{21}	\bar{X}_{21}	\bar{X}_{22}	...	\bar{X}_{1N}	\bar{X}_{2N}
Value of test statistic	T_1		T_2		...	T_N	

Figure 2. The scheme of random sample for a permutation test for paired observations

Source: own elaboration on the basis on Kończak, 2016

This permutation test may then be recursively used for the analysis of the experimental design results, as an alternative for the paired t test.

5. The application of permutation tests in the analysis of experimental results

The application of permutation tests in the analysis of experimental results will be presented for two empirical data sets. These data apply to the single-factor experiment and the design of the experiment for many factors at different levels.

The analysis of results of the single-factor experiment

The experimental data describe the measures of orifice diameter (factor A) and the amount of radon released in showers (Montgomery, 2001). The data are presented in Table 3.

The aim of the research is to describe the dependence between the amount of radon released and the diameter of orifice. Then the difference between all pairs of experimental trials should be investigated. It is assumed that the significance level is $\alpha = 0.05$.

Table 3. Experimental data

No.	Levels of factor <i>A</i>	Values of response variable				y_i	\bar{y}_i
		1	2	3	4		
1	0.37	80	83	83	85	331	82.75
2	0.51	75	75	79	79	308	77.00
3	0.71	74	73	76	77	300	75.00
4	1.02	67	72	74	74	287	71.75
5	1.40	62	62	67	69	260	65.00
6	1.99	60	61	64	66	251	62.75

Source: Montgomery, 2001

Table 4. The results of Tukey's Test

$\bar{y}_i - \bar{y}_j$	Values of means difference	$\bar{y}_i - \bar{y}_j$	Values of means difference
$\bar{y}_1 - \bar{y}_2$	5.75	$\bar{y}_2 - \bar{y}_6$	14.25*
$\bar{y}_1 - \bar{y}_3$	7.75*	$\bar{y}_3 - \bar{y}_4$	3.25
$\bar{y}_1 - \bar{y}_4$	11.00*	$\bar{y}_3 - \bar{y}_5$	10.00*
$\bar{y}_1 - \bar{y}_5$	17.75*	$\bar{y}_3 - \bar{y}_6$	12.25*
$\bar{y}_1 - \bar{y}_6$	20.00*	$\bar{y}_4 - \bar{y}_5$	6.75*
$\bar{y}_2 - \bar{y}_3$	2.00	$\bar{y}_4 - \bar{y}_6$	9.00*
$\bar{y}_2 - \bar{y}_4$	5.25	$\bar{y}_5 - \bar{y}_6$	2.25
$\bar{y}_2 - \bar{y}_5$	12.00*		

Source: own elaboration.

The analysis of experimental results was prepared with the use of Tukey's Test. The value of test statistic was equal to

$$T_{0.05} \approx q_{0.05}(6.18) \cdot 1.36 = 4.45 \cdot 1.36 = 6.03 .$$

The absolute values of the difference between means were compared with the value of Tukey's test statistics. The results are presented in Table 4.

In the matched pairs with “*”, the means are different, which proves that the orifice diameter in these experimental trials has an impact on the amount of radon released.

Similar considerations were obtained with the use of Fisher's Least Significant Difference Method. The value of test statistics $LSD \approx 3.9981$. The results of the Fisher Least Significant Difference Method are presented in Table 5.

The results for Fisher's Least Significant Difference Method are slightly different from Tukey's test results. Fisher's Least Significant Difference Method indicates two pairs of experimental trials in which the means between the response variable are different.

In the same case, a permutation test was used. The test statistic (9) was considered and the permutation test was conducted for all pairs of experimental trials. The estimated values of ASL are presented in Table 6.

Table 5. The results of Fisher's Least Significant Difference Method.

$\bar{y}_i - \bar{y}_j$	Values of means difference	$\bar{y}_i - \bar{y}_j$	Values of means difference
$\bar{y}_1 - \bar{y}_2$	5.75*	$\bar{y}_2 - \bar{y}_6$	14.25*
$\bar{y}_1 - \bar{y}_3$	7.75*	$\bar{y}_3 - \bar{y}_4$	3.25
$\bar{y}_1 - \bar{y}_4$	11.00*	$\bar{y}_3 - \bar{y}_5$	10.00*
$\bar{y}_1 - \bar{y}_5$	17.75*	$\bar{y}_3 - \bar{y}_6$	12.25*
$\bar{y}_1 - \bar{y}_6$	20.00*	$\bar{y}_4 - \bar{y}_5$	6.75*
$\bar{y}_2 - \bar{y}_3$	2.00	$\bar{y}_4 - \bar{y}_6$	9.00*
$\bar{y}_2 - \bar{y}_4$	5.25*	$\bar{y}_5 - \bar{y}_6$	2.25
$\bar{y}_2 - \bar{y}_5$	12.00*		

Source: own elaboration.

Table 6. The estimated values of ASL

$\bar{Y}_i - \bar{Y}_j$	ASL	$\bar{Y}_i - \bar{Y}_j$	ASL
$\bar{Y}_1 - \bar{Y}_2$	0.030*	$\bar{Y}_2 - \bar{Y}_6$	0.031*
$\bar{Y}_1 - \bar{Y}_3$	0.020*	$\bar{Y}_3 - \bar{Y}_4$	0.194
$\bar{Y}_1 - \bar{Y}_4$	0.026*	$\bar{Y}_3 - \bar{Y}_5$	0.035*
$\bar{Y}_1 - \bar{Y}_5$	0.023*	$\bar{Y}_3 - \bar{Y}_6$	0.037*
$\bar{Y}_1 - \bar{Y}_6$	0.033*	$\bar{Y}_4 - \bar{Y}_5$	0.083

$\bar{Y}_i - \bar{Y}_j$	ASL	$\bar{Y}_i - \bar{Y}_j$	ASL
$\bar{Y}_2 - \bar{Y}_3$	0.264	$\bar{Y}_4 - \bar{Y}_6$	0.038*
$\bar{Y}_2 - \bar{Y}_4$	0.019*	$\bar{Y}_5 - \bar{Y}_6$	0.387
$\bar{Y}_2 - \bar{Y}_5$	0.027*		

Source: own elaboration

It is important to note that the results of the permutation test, in contrast to Tukey’s Test and the Fisher Least Significant Method, indicate that the means of variables Y_4 and Y_5 are different.

The analysis of the result of the design of the experiment including two factors at a different number of levels

The experimental data presented in Table 7 refer to the analysis of the dependence between surface of metal (response variable Y) and the two factors: the feed rate (X_1) and the depth of cut (X_2) (Montgomery, 2001). Three replications of the experiment were prepared.

Table 7. The results of the conducted experiment including two factors at three and four levels.

No.	X_1	X_2	Values of response variable		
			1	2	3
1	0.2	0.15	74	64	60
2	0.2	0.18	79	68	73
3	0.2	0.2	82	88	92
4	0.2	0.25	99	104	96
5	0.25	0.15	92	86	88
6	0.25	0.18	98	104	88
7	0.25	0.2	99	108	95
8	0.25	0.25	104	110	99
9	0.3	0.15	99	98	102
10	0.3	0.18	104	99	95
11	0.3	0.2	108	110	99
12	0.3	0.25	114	111	107

Source: Montgomery, 2001

The aim of the investigation is to determine whether the unknown factors have an influence on the response variable in the particular replications. Therefore, it is important to verify whether the means of the response variable in the particular replications of the experiment are equal. Moreover, in order not to lose the information included in the experimental results, the paired observations in the particular experimental trials should be taken into account. For this purpose,

the permutation test for a comparison of the two variable means for paired observations was used. The hypothesis (4) and the test statistic (9) are considered. The results of this permutation test are presented in Table 8.

Table 8. The ASL values for the permutation test for paired observations.

Y_i	Y_j	<i>ASL</i>
Y_1	Y_2	0.968
Y_1	Y_3	0.027
Y_2	Y_3	0.046

Source: own elaboration

On the basis of the permutation test results, it can be stated that the means of response variable in the third replication are different from the means of response variable in the other replications. Therefore, it is possible to say that in the third replication of the experiment the unknown factor has an impact on the response variable.

The permutation tests used in this chapter do not require the fulfilment of the assumptions about the distribution of the response variable and allow for an analysis of the experimental results using the experimental data only. The results of the performed analysis with classical statistical methods and permutation methods lead to similar results, but the permutation methods are more reasonable because of the small number of samples.

6. Conclusions

In the process of experimental design, classical statistical methods are used; their results are estimated on the basis of theoretical distributions and depend on the sample size. Moreover, the possibility of application of classical statistical methods is limited due to the specific assumptions. Therefore, it is well-justified to look for statistical methods based on empirical data only which can be a supplement to the analysis of experimental results.

In this article, two types of experimental designs have been presented: the single factor experiment and the experiment with two factors at a different number of levels. In both cases, the number of experimental trials is small, so it is possible that the assumptions applying to the distribution of the response variable are not fulfilled. Then the use of classical tests of comparison of means can be unjustified. Therefore another method of comparison of experimental results should be found.

The possibility of the implementation of permutation tests in the analysis of experimental results has been presented in the paper. For the first type of experiment (single factor experiment), the permutation test for comparing means of the response variable in individual experimental trials was used, and in the other case (the experiment includes two factors at a different number of levels), the permutation test for comparing means with the paired observation was used. The use of permutation tests, based on experimental data only, enables the proper analysis of experimental results when the assumption on the distribution of the response variable was not fulfilled.

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O wykorzystaniu testów permutacyjnych w analizie wyników eksperymentów czynnikowych

Streszczenie: Metody planowania eksperymentów są wykorzystywane w statystycznej kontroli jakości procesu produkcyjnego. Właściwe planowanie eksperymentów przed realizacją procesu produkcyjnego prowadzi do poprawy jego rezultatów technologicznych, co w efekcie powoduje poprawę rezultatów ekonomicznych procesu. W ostatnich latach na znaczeniu zyskały metody repróbokowania, wykorzystujące symulacje komputerowe. Jedną z nich są testy permutacyjne służące do weryfikacji hipotez statystycznych. W porównaniu do testów parametrycznych nie wymagają one speł-

nienia restrykcyjnych założeń i mogą być stosowane do niewielkiej liczby obserwacji. Przedmiotem artykułu jest wskazanie możliwości wykorzystania testów permutacyjnych w analizie wyników eksperymentu. Rozważania przeprowadzone zostały dla danych dotyczących rezultatów ustalonego procesu produkcyjnego.

Słowa kluczowe: test Tukeya, test Fishera, planowanie eksperymentów, testy permutacyjne

JEL: C99, C12, C15

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