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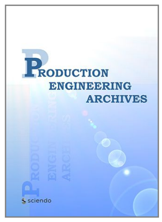

The Response Surface Methodology revisited – comparison of analytical and non-parametric approaches

Przemysław Osocha[1], **Jordan Podgórski**[1]

[1] Cracow University of Technology, Faculty of Mechanical Engineering, Al. Jana Pawła II 37, 31-864 Kraków, Poland
e-mail: przemyslaw.osocha@mech.pk.edu.pl

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Abstract
Since G.E.P. Box introduced central composite designs in early fifties of 20th century, the classic design of experiments (DoE) utilizes response surface models (RSM), however usually limited to the simple form of low-degree polynomials. In the case of small size datasets, the conformity with the normal distribution has very weak reliability and it leads to very uncertain assessment of a parameter statistical significance. The bootstrap approach appears to be better solution than – theoretically proved but only asymptotically equal – *t* distribution based evaluation. The authors presents the comparison of the RSM model evaluated by a classic method and bootstrap approach.

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1. Introduction

In the second half of the twentieth century, industry remained under constant pressure to improve its products. In the last two decades, there has been an additional demand from consumers that these products are new or have completely new functional characteristics. Ignoring these demands leads inevitably to marginalization of the company or pushing it out of the market. On the other hand, conducting research and development is very expensive and involves a high risk of failure. Any tools that increase the effectiveness of these works and reduce the level of risk are highly desirable.

One of the toolset, supporting engineers and researchers, is a design and analysis of experiments (DoE) methodology (Kempthorne and Hinkelmann, 2007; Montgomery, 2008), whose first ideas come from Fisher (Fisher, 1925). It contains many different approaches, optimized to investigate specific objects and processes. They focus mainly on statistical aspects, but also on organizational ones.

The basic feature of the tested object, which differentiates available analytical methods, is the method of setting the value of controlled factors. Setting values can be discrete, stepwise (e.g. type of material, dosage with tablets, supplier, type of part) or continuous (e.g. temperature setting, weight dosing, timing of reaction time). The first group of problems are located in the factorial approach, while the second – in the response surface approach (the well-known acronym: RSM – response surface methodology). The basics of RSM was developed by Box in 1951 (Box and Wilson, 1951), while two duets: Robbins with Monroe (Robbins and Monroe, 1951) and Kiefer with Wolfowitz (Kiefer and Wolfowitz, 1952) created a supporting mathematical formalism.

The general concept of this approach bases on the best identification of the assumed mathematical model while a number of experimental tests is predetermined. This obviously leads to the question: where should the test points be located in the space of controlled factors to achieve the best possible identification of the selected model. These test location schemes are developed by statisticians and known as experimental designs (Montgomery, 2008). From the mathematical point of view, such a problem is almost identically as in the approximation nodes selection e.g. Tschebyshev, Gauss etc. The most popular method of the model identification is least squares method (Gentle and Hardle, 2012), which assume a normal distribution of the random term with a mean equal to zero and an unknown variance. This assumption is very strong and should a posteriori verified. It is usually done by a test of the normality e.g. Kolmogorov-Smirnov (Kolmogorov, 1933; Smirnov, 1948), Anderson-Darling (Anderson and Darling, 1952) or Shapiro-Wilk (Shapiro and Wilk, 1965). If the selected test does not reject, it is good and the predicted response uncertainty may be estimated by typical asymptotic t distribution. But what to do, if it fails? The possible solution is a non-parametric approach which bases on the resampling scheme introduced by Efron (Efron, 1979).

2. A bootstrap concept – short description

The first idea of the bootstrap was introduced by Efron (Efron, 1979) derived from the jackknife procedure developed by Quenouille (Quenouille, 1949) and expanded by Tukey (Tukey, 1958). The approach treats drawings taken from the raw dataset as a source of true measurements. Resampled datasets are analyzed and functions of interest are evaluated giving the bootstrapped distributions, treated as derived from truly replicated measurements. In a particular case, the model identification procedure may be the evaluated function.

Such approach is iterated many times, typically from thousands to millions, and results are collected. Then, the obtained dataset is analyzed and distributions of selected statistics are numerically identified, especially their means and quasi-empirical confidence intervals.

3. Statistical significance in bootstrapped RSM model

Pietraszek and Wojnar (Pietraszek and Wojnar, 2016) showed how to assessed numerically statistical significance of RSM model parameters without any attempt to typical t distribution based methods.

The classic sequence (raw dataset, statistic evaluation, statistical test, p-value, comparison to alpha) was replaced with (raw dataset, bootstrap, bootstrapped datasets, set of statistics, histogram, alpha/2-tails, check for zero in bounds). It means that bootstrap was a procedure to obtain quasi-empirical confidence interval based truncated on alpha/2 tails. Then, the intervals was checked whether contains zero value inside. If yes – the statistic is insignificant; if not – the statistic is significant. The position of zero relative to the center of the interval gives the well-known p value.

Pietraszek and Wojnar (Pietraszek and Wojnar, 2016) analyzed the dataset obtained from the investigation of the vertebrae strength, however it may easily generalized into any analogous technological problem. The outcome (a strength of vertebrae) was dependent on three observed factors, specific properties of the vertebrae structure: a density of trabecular bone, a number of branches in a trabecular bone and a number of junctions on the branches in trabecular bone. The source dataset was small and it had only 23 records. It was enough to identify a linear prediction model, but it was inadequate to achieve a strong estimation of a uncertainty. They used a specific bootstrap variant described by Shao and Tu (Shao and Tu, 1995):

a) the original dataset is used to identify a predictive model,
b) the model is evaluated on the original data set and residual values are obtained,
c) the residuals dataset is resampled and drawn values are added to model predictions – they create a new dataset of outcome,
d) the new outcome dataset combined with original factors is used to identify a bootstrapped model – obtained bootstrapped parameters are collected.

The steps (c) and (d) are iterated thousands and thousands times, and huge dataset of collected parameters is built. Pietraszek and Wojnar (Pietraszek and Wojnar, 2016) used the approach mentioned above and obtained a complete distributions of the model parameters. Then, their 95% confidence intervals were evaluated. Their basic RSM model was constructed as:

$$R_c = b_{const} + b_{BV/TV} \cdot BVTV + b_{branches} \cdot Branches + \\ + b_{Junctions} \cdot Junctions \qquad (1)$$

where:
R_c – observed strength of a vertebrae
b_{const} – constant term,
$b_{BV/TV}$ – coefficient of relative density of a trabecular bone,
$b_{branches}$ – coefficient of a average number of branches in trabecular bone,
$b_{junctions}$ – coefficient of a average number of junctions on the branches in trabecular bone.

The replication of this model based on the data included in the article (Pietraszek and Wojnar, 2016) led to the dataset of bootstrapped parameters of the Eq.1. The data were tested for normality and revealed that data distributions are far from normality. The parameter b_{const} has mean 0.2823 while the classically evaluated is 0.34. Its shape is explicitly non-normal (Fig. 1).

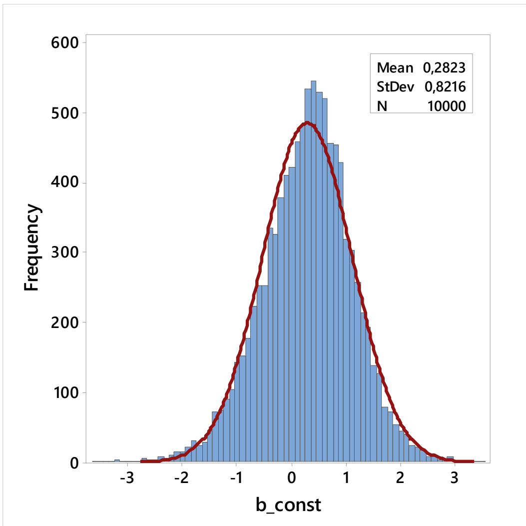

Fig. 1. Histogram of bootstrapped b_{const} parameter

The test of normality shows (Fig. 2) that p-value is less than 0.01 i.e. the normality of the parameter is rejected.

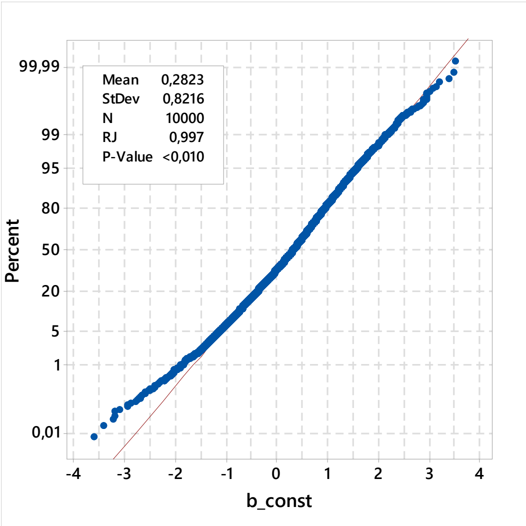

Fig. 2. The probability plot of bootstrapped b_{const} parameter

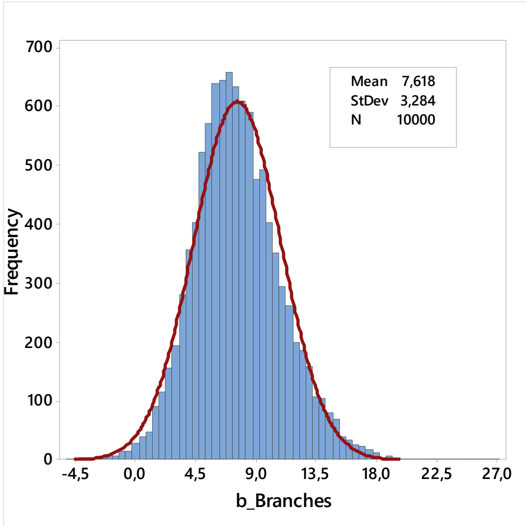

Fig. 5. Histogram of bootstrapped $b_{Branches}$ parameter

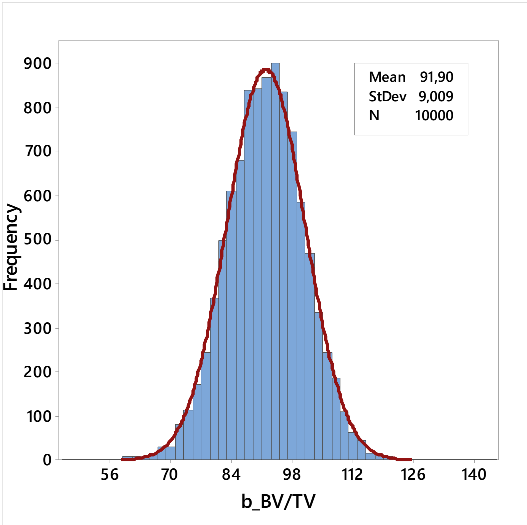

Fig. 3. Histogram of bootstrapped $b_{BV/TV}$ parameter

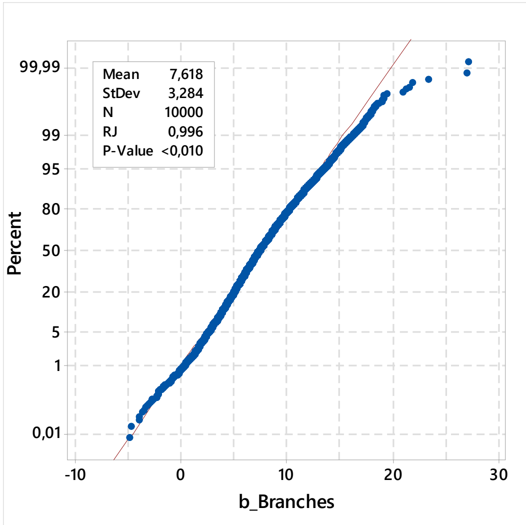

Fig. 6. The probability plot of bootstrapped $b_{Branches}$ parameter

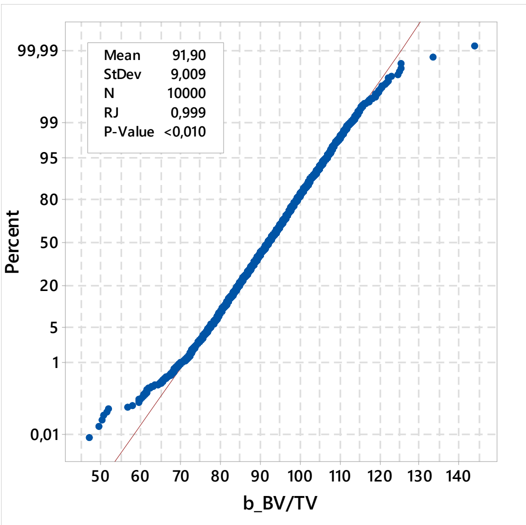

Fig. 4. The probability plot of bootstrapped $b_{BV/TV}$ parameter

The parameter $b_{BV/TV}$ has mean 91.90 while the classically evaluated is 92.61. Its shape is not so explicitly not-normal (Fig. 3) as the previous one, but the test of normality was rejected also (Fig. 4).

The parameter $b_{Branches}$ has mean 7.62 while the classically evaluated is 7.26. Its shape is explicitly not-normal (Fig. 5) and the test of normality was rejected also (Fig. 6).

Finally, the parameter $b_{Junctions}$ has mean -13.74 while the classically evaluated is -13.16. Its shape is explicitly not-normal (Fig. 7) and the test of normality was rejected (Fig. 8).

One can observe that all distributions are not-normal, their means are different than those evaluated classically and, additionally, three distributions (Fig. 1, Fig.5 and Fig. 7) have a distinct skewness. It shows that a classic model, based on assumptions that are not met, leads to not very accurate results. The non-parametric approach using the bootstrap method allows to create the whole-distribution-based statistics, not only t distribution based asymptotic one, loosely related to the real data.

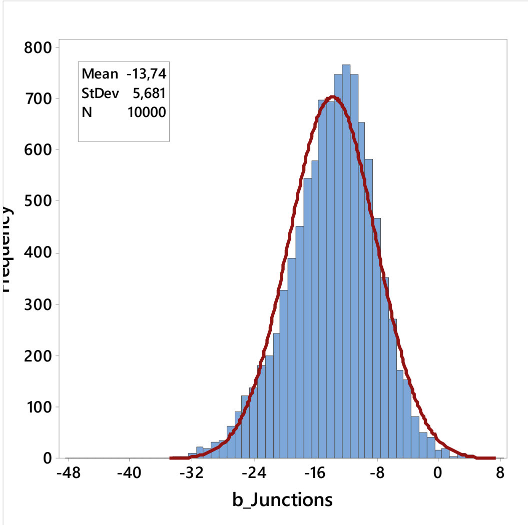

Fig 7. Histogram of bootstrapped $b_{Branches}$ parameter

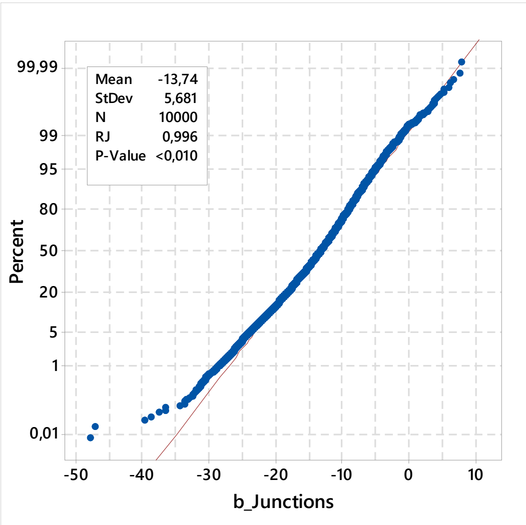

Fig. 8. The probability plot of bootstrapped $b_{Junctions}$ parameter

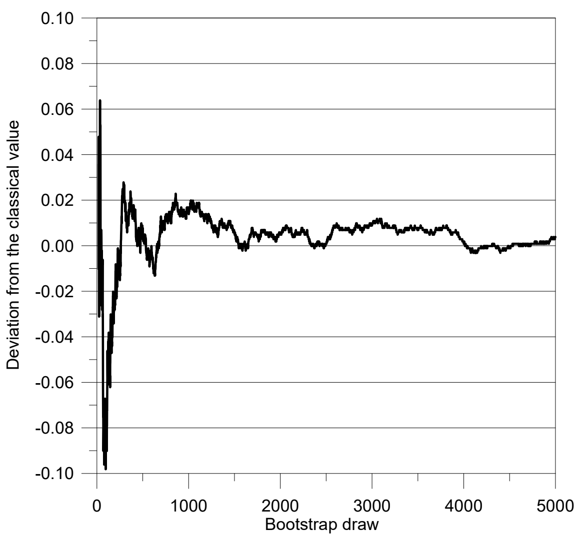

Fig 9. The deviation of a bootstrapped parameter from a perfect value (source: Osocha et. al., 2015)

An interesting question is what should be the number of iterations in the bootstrap method. Such problem was addressed (Osocha et al., 2015) and the stabilization of results appeared only above 4000…5000 iterations.

4. Conclusions

The comparison of the classically evaluated RSM model and the bootstrap based approach was presented. The difference between results obtained from LSQ with normality assumption and – in contrast – the bootstrap based non-parametric approach was showed.

Bootstrap approach appears to be effective computational method to identify parameters of RSM effects model and their statistical properties and – additionally – it does not require to make a priori inconvenient assumptions.

The bootstrap approach appears to be an effective and easy-to-use procedure. However, it should be emphasized that this approach requires careful and continuous watching at residual plot to detect breakdown iterations which stabilizes bootstrap means.

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自动驾驶汽车的不规则操作

關鍵詞
事故重建，自动驾驶汽车，
自驾车
紧急
车辆运动模拟

摘要
今天，随着车辆自主功能的普及，强调了引发事故的责任。自导功能在某些交通情况下起作用，但事故发生，因此，下面的文章提出了对该问题的分析。其目的是表明具有自动驾驶功能的车辆不能提供车辆制造商建议的驾驶员安全水平。在这篇文章中，最近的四个事件和一个分析是否可以避免这些事故是一个人类驱动因素，或者它们是如何发生的，具有适当的自我驱动功能。在每个调查的案例中，涉及具有自驱动功能的车辆。在对事故的评估和评估的基础上，得出结论，当前的自行式车辆是否提供了驾驶员和社会对这些车辆的期望。
在车辆模拟程序的帮助下说明事故过程的重建，特别强调所得到的参数，特别是避免事故。