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Statistical inference on repeated regular two-level factorial experiments

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Abstract: **In this paper, we proposed two methods for hypothesis tests on the active effect that effect the mean of the response in the replicated regular two-level factorial experiments. The first method was proposed based on bootstrap, and the second method was proposed based on student's t test. Simulation results show that the two approaches have better control rate under the small sample size.**

Keywords: Bootstrap; Student's t test; Control Rate; Factorial experiment

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1. Introduction

In the field of medicine, replicated regular two-level factorial experiments are mostly used to screen the best treatment and drug formulation. These experiments are also widely used in industry (Box[1] (1978)). Identify active effects that affects the mean of the response by analyzing the response in these experiments.

In a two-level factorial experiment, let y_{ij} be the response for the j th tentative repeated in the i th tentative, $i=1,\cdots,m$ and $j=1,\cdots,n_i$. Here y_{ij} 's are independent. Suppose that the number of data obtained for each tentative is n, that is $n_1=\cdots=n_m=n$. Assume that there are I factors of influence. Let x_{ik} be the level value of the k th influence factor for the i th tentative, and x_{ik} is equal to 1 or -1, $k=1,\cdots,I$.

In this paper, the model we utilize for modeling the mean of the response is normal model with a linear regression for the mean (Wu[2] (2000), Loughin[3] (2011)). We call this model the location model. Let the response distribution be the normal distribution, which is

$$y_{ij} \sim N\left(\mu_i,\sigma_i^2\right),\ i=1,\cdots,m,\ j=1,\cdots,n, \tag{1}$$

and the location model is

$$\mu_i=\alpha_0+\alpha_1 x_{i1}+\cdots+\alpha_I x_{iI},\ i=1,\cdots,m. \tag{2}$$

From (1) and (2), we get the least square estimators of $\alpha_1,\cdots,\alpha_I$

$$\hat{\alpha}_k=\frac{1}{m}x_k'\bar{Y}=\frac{1}{m}\sum_{i=1}^{m}x_{ik}\bar{y}_{i\cdot},\ k=1,\cdots,I, \tag{3}$$

where $\bar{y}_{i\cdot}=\frac{1}{n}\sum_{j=1}^{n}y_{ij}$, $\bar{Y}=\left(\bar{y}_{1\cdot},\cdots,\bar{y}_{m\cdot}\right)'$ and $x_k=\left(x_{1k},\cdots,x_{mk}\right)'$, $k=1,\cdots,I$, x_k has $\frac{m}{2}$ elements equal to 1 and another $\frac{m}{2}$ elements equal to -1, and $x_s'x_t=0\left(s\neq t\right)$.

Under (1) and (3), we have

$$E\left(\hat{\alpha}_k\right)=E\left(\frac{1}{m}\sum_{i=1}^{m}x_{ik}\bar{y}_{i\cdot}\right)=\frac{1}{m}\sum_{i=1}^{m}x_{ik}\mu_i=\alpha_k,$$

$$Var\left(\hat{\alpha}_k\right)=\frac{1}{m}x_k'Var\left\{\left(\bar{y}_{1\cdot},\cdots,\bar{y}_{m\cdot}\right)'\right\}x_k=\frac{1}{m^2n}\sum_{i=1}^{m}\sigma_i^2,$$

as a result, that $\hat{\alpha}_k$ obeys the distribution

$$\hat{\alpha}_k \sim N\left(\alpha_k,\frac{1}{m^2n}\sum_{i=1}^{m}\sigma_i^2\right),\ k=1,\cdots,I. \tag{4}$$

In this paper, we consider the null hypothesis H_0: $\alpha_k=0$. Based on the location model, several hypothesis test methods have been proposed, such as t-type statistic method (Wu[2] (2000)), jackknife method (Variyath[4] (2005)). However, these methods are either too radical or conservative in some cases. In this article, we conduct hypothesis tests on the active effect to identify active effects that affects the mean of the response by bootstrap and student's t test under the normal assumption. The rest of the article is organized as follows. In Section 2, the bootstrap method and its calculation steps are introduced. In Section 3, we propose the student's t test method for testing the null hypothesis. In Section 4, we use Monte Carlo method to analyze the advantages and disadvantages of the two methods. In Section 5, we give some conclusions.

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2. Bootstrap Method

Efron[5](1979) proposed the Bootstrap method of statistical inference, which is widely used. Bootstrap method was used by Cheng[6](1995) in computer simulation. Below we will introduce bootstrap method how to deal with the problem of this article.

Let $s_i^2=\frac{1}{n-1}\sum_{j=1}^{n}\left(y_{ij}-\bar{y}_{i\cdot}\right)^2$, i=1,⋯, m , then for the given statistic s_i^2, we have

$$\frac{(n-1)s_i^2}{\sigma_i^2}\sim\chi_{n-1}^2 . \tag{5}$$

From (4) and (5), under the condition that the null hypothesis H_0: $\alpha_k=0$ is established, we propose a t-type test statistic

$$t_k^0=\frac{\hat{\alpha}_k}{\sqrt{\frac{1}{m^2n}\sum_{i=1}^{m}s_i^2}},\ k=1,\cdots,I .$$

The observed values $\hat{\alpha}_{Bk}$ and s_{Bi}^2 of the given bootstrap sample are generated by $N\left(\hat{\alpha}_k,\frac{1}{m^2n}\sum_{i=1}^{m}s_i^2\right)$ and $\frac{s_i^2}{n-1}\chi_{n-1}^2$ respectively. Let $U_k\overset{def}{=}N(0,1)$, $V_i\overset{def}{=}\chi_{n-1}^2$, we obtain

$$\hat{\alpha}_{Bk}\overset{def}{=}\hat{\alpha}_k+U_k\sqrt{\frac{1}{m^2n}\sum_{i=1}^{m}s_i^2},\ s_{Bi}^2\overset{def}{=}\frac{s_i^2}{n-1}V_i .$$

Therefore, the bootstrap pivotal quantity for $t_k=\frac{\hat{\alpha}_k-\alpha_k}{\sqrt{\frac{1}{m^2n}\sum_{i=1}^{m}s_i^2}}$ is

$$t_{Bk}=\frac{\hat{\alpha}_{Bk}-\hat{\alpha}_k}{\sqrt{\frac{1}{m^2n}\sum_{i=1}^{m}s_{Bi}^2}}=\frac{U_k}{\sqrt{\frac{1}{n-1}\sum_{i=1}^{m}\left(\frac{s_i^2}{\sum_{i=1}^{m}s_i^2}\right)V_i}},$$

t_{Bk} is the same as the t-type test statistic constructed by P.Li et al. [7](2019).

Then we could test the null hypothesis H_0: $\alpha_k=0$ by bootstrap method. The algorithm of bootstrap method shows as follows.

Step 1. Generate n samples in the i th experiment, calculate the variance of these samples s_i^2,i=1,⋯,m .

Step 2. Generate a random variable $U_k\sim N(0,1)$.

Step 3. Generate m independent random variable $V_i\sim\chi_{n-1}^2$, i=1,⋯, m .

Step 4. Compute $t_{Bk}=\frac{U_k}{\sqrt{\frac{1}{n-1}\sum_{i=1}^{m}\left(\frac{s_i^2}{\sum_{i=1}^{m}s_i^2}\right)V_i}}$.

Step 5. Repeat step 2 and step 4 M times to obtain M values of t_{Bk}, recorded as $t_{Bk,1},\cdots,t_{Bk,M}$.

Step 6. Compute the generalized p-value $p=2\min\left(P\left(t_{Bk}\ge t_k^0\right),P\left(t_{Bk}\le t_k^0\right)\right)$.

For the given α value, we reject H_0: $\alpha_k=0$ if $p\ge\alpha$.

3. Student's t test Method

With (1), we have

$$\bar{y}_{\cdot j}\sim N\left(\frac{1}{m}\sum_{i=1}^{m}\mu_i,\frac{1}{m^2}\sum_{i=1}^{m}\sigma_i^2\right),$$
$$\sum_{i=1}^{m}\left(\bar{y}_{\cdot j}-\bar{y}\right)^2\sim\left(\frac{1}{m^2}\sum_{i=1}^{m}\sigma_i^2\right)\chi_{n-1}^2 , \tag{6}$$

where $\bar{y}_{\cdot j}=\frac{1}{m}\sum_{i=1}^{m}y_{ij}$, $\bar{y}=\frac{1}{mn}\sum_{i=1}^{m}\sum_{j=1}^{n}y_{ij}$.

From (4) and (6), under the assumption that the null hypothesis H_0: $\alpha_k=0$ is established, it is easy to know that

$$\frac{\hat{\alpha}_k}{\sqrt{\frac{1}{m^2n}\sum_{i=1}^{m}\sigma_i^2}}\sim N(0,1),\ \frac{m^2\bar{s}^2}{\sum_{i=1}^{m}\sigma_i^2}\sim\chi_{n-1}^2 ,$$

where $\bar{s}^2=\sum_{j=1}^{n}\left(\bar{y}_{\cdot j}-\bar{y}\right)^2$. So, we could construct a t-type test statistic

$$T_k=\frac{\frac{\hat{\alpha}_k}{\sqrt{\frac{1}{m^2n}\sum_{i=1}^{m}\sigma_i^2}}}{\sqrt{\frac{m^2\bar{s}^2}{\sum_{i=1}^{m}\sigma_i^2}\Big/(n-1)}}=\frac{\hat{\alpha}_k}{\sqrt{\frac{1}{n(n-1)}\bar{s}^2}}\sim t_{n-1},\ k=1,\cdots,I .$$

For the given α value, we reject H_0: $\alpha_k=0$ if $|T_k|>t_{n-1,1-\alpha/2}$.

4. Simulation Study

In this section, Monte Carlo simulation study is used to analyze the performance of the two methods described in Section 2 and Section 3. We compare bootstrap method (BM) with student's t test method (TM). The criterion is whether to control the individual error rate at the given α value.

In the simulation study, we conduct simulations of 2^2, 2^3 and 2^4 experiments. For the 2^2 experiment with 2 two-level factors, A and B, the values of A, B,

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AB are equal to 1 or -1 depending on the combination of factor levels. For the 2^3 experiment with 3 two-level factors, A, B, and C, the values of A, B, C, AB, AC, BC, ABC are equal to 1 or -1 depending on the combination of factor levels. For the 2^4 experiment with 4 two-level factors, A, B, C, and D, the values of A, B, C, D, AB, AC, AD, BC, BC, BD, CD, ABC, ABD, ACD, BCD, and ABCD are equal to 1 or -1 depending on the combination of factor levels.

Let $\alpha=0.05$, the simulation study using the following steps:

Step 1. Generate sample from $N(\mu_i,\sigma_i^2)$, i=1,⋯,m.

Step 2. Test the null hypothesis by BCI and TM respectively. Where the simulation size of BCI is M=50000.

Step 3. Repeat steps 1 and 2 20000 times, calculate the rates of rejection of the null hypothesis.

For $\alpha=0.05$, we consider two cases of homoscedasticity and heteroskedasticity in each factorial experiment. From tables 1-6, we get the following results.

(a) In all cases, student's t test method controls the rates of rejection of the null hypothesis around 0. 05.

(b)When n is small, for example, n=2, the bootstrap method is conservative in the case of homogeneity or heteroscedasticity. In other cases, bootstrap method controls the rates of rejection of the null hypothesis around 0.05.

Table 1. Rates of rejection of the null hypothesis for model $y_{ij} \sim N(3+A+0.6B,1)$ in the 2^2 experiment

	BM					TM				
Effect	n=2	n=3	n=4	n=5	n=6	n=2	n=3	n=4	n=5	n=6
A	0. 3846	0. 8081	0. 9463	0. 9855	0. 9963	0. 1708	0. 4683	0. 7497	0. 9072	0. 9705
B	0. 0247	0. 0380	0. 0409	0. 0452	0. 0462	0. 0494	0. 0525	0. 0466	0. 0486	0. 0491
AB	0. 1577	0. 3925	0. 5679	0. 6911	0. 7894	0. 1072	0. 2287	0. 3831	0. 5326	0. 6561

Table 2. Rates of rejection of the null hypothesis for model $y_{ij} \sim N(2+0.6B+AB,\exp(0.5B+0.3AB))$ in the 2^2 experiment

	BM					TM				
Effect	n=2	n=3	n=4	n=5	n=6	n=2	n=3	n=4	n=5	n=6
A	0. 0332	0. 0406	0. 0449	0. 0503	0. 0474	0. 0508	0. 0485	0. 0518	0. 0516	0. 0490
B	0. 1464	0. 3397	0. 4928	0. 6124	0. 7139	0. 1005	0. 2068	0. 3385	0. 4692	0. 5892
AB	0. 3545	0. 7204	0. 8935	0. 9602	0. 9867	0. 1616	0. 4261	0. 6933	0. 8631	0. 9463

Table 3. Rates of rejection of the null hypothesis for model $y_{ij} \sim N(6+0.6A+B+0.3AB,1)$ in the 2^3 experiment

	BM					TM				
Effect	n=2	n=3	n=4	n=5	n=6	n=2	n=3	n=4	n=5	n=6
A	0. 4214	0. 7576	0. 8924	0. 9521	0. 9804	0. 1468	0. 3797	0. 6249	0. 8051	0. 9039
B	0. 8630	0. 9930	0. 9996	0. 9990	1. 0000	0. 2459	0. 7050	0. 9488	0. 9952	0. 9995
C	0. 0273	0. 0399	0. 0459	0. 0460	0. 0468	0. 0484	0. 0519	0. 4735	0. 0485	0. 0514
AB	0. 1185	0. 2450	0. 3497	0. 4461	0. 5169	0. 0796	0. 1463	0. 2205	0. 3110	0. 3879
AC	0. 0282	0. 0402	0. 0486	0. 0468	0. 0509	0. 0486	0. 0506	0. 0506	0. 0485	0. 0523
BC	0. 0287	0. 0404	0. 0469	0. 0473	0. 0497	0. 0486	0. 0493	0. 0501	0. 0483	0. 0487
ABC	0. 0272	0. 0396	0. 0461	0. 0468	0. 0472	0. 0495	0. 0505	0. 0486	0. 0462	0. 0500

Table 4. Rates of rejection of the null hypothesis for model $y_{ij} \sim N(9+0.6A+0.3B+0.6AC,\exp(0.6B+C+0.3AB))$ in the 2^3 experiment

	BM	TM

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Effect	n=2	n=3	n=4	n=5	n=6	n=2	n=3	n=4	n=5	n=6
A	0. 1753	0. 3254	0. 4568	0. 5534	0. 6528	0. 0969	0. 1875	0. 3043	0. 4084	0. 5265
B	0. 0893	0. 1472	0. 1980	0. 2483	0. 2934	0. 0687	0. 1013	0. 1440	0. 1906	0. 2354
C	0. 0404	0. 0471	0. 0460	0. 0474	0. 0475	0. 0518	0. 0498	0. 0476	0. 0497	0. 0501
AB	0. 0435	0. 0459	0. 0470	0. 0460	0. 0509	0. 0515	0. 0495	0. 0498	0. 0494	0. 0506
AC	0. 2346	0. 4410	0. 6059	0. 7133	0. 8076	0. 1122	0. 2429	0. 4018	0. 5443	0. 6762
BC	0. 0395	0. 0475	0. 0499	0. 0478	0. 0524	0. 0520	0. 0488	0. 0507	0. 0488	0. 0527
ABC	0. 0438	0. 0449	0. 0481	0. 0447	0. 0496	0. 0534	0. 0487	0. 0517	0. 0510	0. 0494

Table 5. Rates of rejection of the null hypothesis for model $y_{ij} \sim N(6+0.2A+0.4B+0.4AC+0.3CD,1)$ in the 2^4 experiment

	BM					TM				
Effect	n=2	n=3	n=4	n=5	n=6	n=2	n=3	n=4	n=5	n=6
A	0. 1387	0. 2488	0. 3402	0. 4152	0. 4855	0. 0780	0. 1346	0. 2012	0. 2752	0. 3562
B	0. 4774	0. 7482	0. 8761	0. 9381	0. 9718	0. 1404	0. 3483	0. 5801	0. 7594	0. 8764
C	0. 0336	0. 0426	0. 0476	0. 0485	0. 0481	0. 0518	0. 0491	0. 0509	0. 0486	0. 0481
D	0. 0317	0. 0428	0. 0448	0. 0495	0. 0474	0. 0494	0. 0489	0. 0483	0. 0506	0. 0508
AB	0. 0334	0. 0448	0. 0476	0. 0454	0. 0491	0. 0515	0. 0483	0. 0485	0. 0485	0. 0491
AC	0. 4807	0. 7497	0. 8703	0. 9429	0. 9722	0. 1407	0. 3494	0. 5761	0. 7628	0. 8762
BC	0. 0331	0. 0444	0. 0486	0. 0465	0. 0475	0. 0490	0. 0487	0. 0507	0. 0493	0. 0507
AD	0. 0322	0. 0436	0. 0466	0. 0481	0. 0458	0. 0486	0. 0490	0. 0497	0. 0480	0. 0477
BD	0. 0343	0. 0447	0. 0450	0. 0475	0. 0497	0. 0511	0. 0486	0. 0491	0. 0500	0. 0487
CD	0. 2882	0. 4968	0. 6452	0. 7468	0. 8278	0. 1078	0. 2277	0. 3809	0. 5282	0. 6590
ABC	0. 0319	0. 0449	0. 0465	0. 0477	0. 0508	0. 0489	0. 0487	0. 0489	0. 0479	0. 0497
ABD	0. 0303	0. 0442	0. 0452	0. 0493	0. 0492	0. 0501	0. 0486	0. 0482	0. 0499	0. 0509
ACD	0. 0321	0. 0432	0. 0464	0. 0485	0. 0487	0. 0505	0. 0483	0. 0491	0. 0471	0. 0477
BCD	0. 0303	0. 0442	0. 0467	0. 0468	0. 0514	0. 0505	0. 0491	0. 0485	0. 0468	0. 0502
ABCD	0. 0335	0. 0446	0. 0452	0. 0476	0. 0493	0. 0491	0. 0484	0. 0481	0. 0508	0. 0480

Table 6. Rates of rejection of the null hypothesis for model $y_{ij} \sim N(5+0.6A+0.3B+0.6AD+0.3BCD,\exp(A+C+0.3AC+0.BD))$ in the 2^4 experiment

	BM					TM				
Effect	n=2	n=3	n=4	n=5	n=6	n=2	n=3	n=4	n=5	n=6
A	0. 3010	0. 5068	0. 6722	0. 7881	0. 8708	0. 1157	0. 2647	0. 4460	0. 6089	0. 7367
B	0. 1081	0. 1708	0. 2260	0. 2833	0. 3356	0. 0698	0. 1088	0. 1609	0. 2110	0. 2631
C	0. 0455	0. 0445	0. 0477	0. 0475	0. 0484	0. 0492	0. 0499	0. 0497	0. 0505	0. 0496
D	0. 0469	0. 0472	0. 0483	0. 0486	0. 0480	0. 0489	0. 0508	0. 0512	0. 0512	0. 0506
AB	0. 0447	0. 0481	0. 0465	0. 0477	0. 0452	0. 0488	0. 0472	0. 0492	0. 0526	0. 0441
AC	0. 0456	0. 0442	0. 0474	0. 0443	0. 0481	0. 0500	0. 0493	0. 0490	0. 0476	0. 0493
BC	0. 0464	0. 0483	0. 0463	0. 0499	0. 0466	0. 0506	0. 0497	0. 0499	0. 0510	0. 0454
AD	0. 2960	0. 5057	0. 6774	0. 7911	0. 8676	0. 1185	0. 2631	0. 4467	0. 6081	0. 7378
BD	0. 0452	0. 0484	0. 0460	0. 0498	0. 0490	0. 0492	0. 0513	0. 0501	0. 0502	0. 0487
CD	0. 0460	0. 0485	0. 0495	0. 0475	0. 0488	0. 0492	0. 0499	0. 0488	0. 0512	0. 0494
ABC	0. 0458	0. 0486	0. 0475	0. 0492	0. 0476	0. 0497	0. 0494	0. 0488	0. 0511	0. 0449

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ABD	0. 0446	0. 0463	0. 0454	0. 0484	0. 0478	0. 0498	0. 0484	0. 0490	0. 0498	0. 0484
ACD	0. 0445	0. 0480	0. 0470	0. 0469	0. 0499	0. 0492	0. 0495	0. 0490	0. 0507	0. 0500
BCD	0. 1093	0. 1666	0. 2242	0. 2888	0. 3325	0. 0690	0. 1052	0. 1574	0. 2120	0. 2564
ABCD	0. 0466	0. 0467	0. 0462	0. 0462	0. 0452	0. 0497	0. 0490	0. 0479	0. 0502	0. 0505

5. Conclusion

We have proposed two methods for test the null hypothesis based on bootstrap and student's t test. When the sample size n is large, bootstrap method performs well. In this case, we can choose bootstrap method. But student's t test method is less affected by variables, and has a wide range of application. It not only has a good control rate in the case of small sample size n, but also performs well in the case of homogeneity or heteroscedasticity. In conclusion, student's t test method is better than bootstrap method.

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