# Asymptotic expansion for Lack-of-Fit test under nonnormality

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**ABSTRACT.** It is shown that the Lack-of-Fit test can be considered as the likelihood ratio test on the mean structure for some linear model. The asymptotic expansion of the null distribution of the test statistic is derived up to order  $n^{-1}$  under nonnormality. A certain robustness against nonnormality is also investigated.

### 1. Introduction

Lack-of-Fit test is the test to see whether the expectation of response variables is shown as some linear function of explanatory variables when the repeated tests are playable under the appointed explanatory variables. (For example, see [3], pp. 25–27.) It is well-known that the null distribution of the test statistic is F-distribution under the normality of errors. In section 2, we show that the test can be considered as the likelihood ratio test on the mean structure for some linear model. In [4], we obtain an asymptotic expansion of the null-distribution up to order  $n^{-1}$ . Also in this section, we introduce Lack-of-Fit test. In section 3, we derive the asymptotic expansion of null distribution of this test statistic. In section 4, we consider a robustness against nonnormality. In section 5, we give some results of numerical experiments.

## 2. Lack-of-Fit test

Consider the following sets of explanatory variables and response variables.

response 
$$Y$$
  $y_{11} \dots y_{1n_1} \dots y_{j1} \dots y_{jn_j} \dots y_{k1} \dots y_{kn_k}$   
Explanatory  $x$   $x_1 \dots x_1 \dots x_j \dots x_j \dots x_k \dots x_k$ 

Let x be the non-random variable to take the value in  $(x_1, ..., x_k)$ , Y be the response variable, and  $\varepsilon$  be the random variable due to the error with  $E(\varepsilon) = 0$  and  $Var(\varepsilon) = \sigma^2$ . Assume that

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$$Y = \mu(x) + \varepsilon. \tag{2.1}$$

Our intension is to test for (2.1) whether the mean  $\mu(x)$  has some linear structure. For example, we consider a problem of testing the hypothesis

$$H_0: \mu(x) = \theta_1 + \theta_2 x + \dots + \theta_r x^{r-1}, \qquad H_1: \text{not } H_0.$$
 (2.2)

Let  $\bar{y}_i = (1/n_i) \sum_{j=1}^{n_i} y_{ij}$  be the mean of the response variables correspond to the  $x = x_i$ , and let  $\hat{y}_i$  be the predictive value corresponding to  $x = x_i$  under  $H_0$ . Then, the Lack-of-Fit test rejects  $H_0$  for large values of T:

$$T = \frac{\sum_{i=1}^{k} n_i (\bar{y}_i - \hat{y}_i)^2 / (k - r)}{\sum_{i=1}^{k} \sum_{j=1}^{n_i} (y_{ij} - \bar{y}_j)^2 / (n - k)},$$
(2.3)

where  $\hat{y}_i$  is the predicted value corresponding to  $x_i$  given by the usual least squares method under the hypothesis  $H_0$ .

Define  $\mathbf{1}_m = (1, \dots, 1)'$   $(m \times 1 \text{ vector})$  for arbitrary positive integer m, and

$$L = \begin{pmatrix} \mathbf{1}_{n_1} & O \\ & \ddots & \\ O & & \mathbf{1}_{n_k} \end{pmatrix}, \qquad X = \begin{pmatrix} x_1 & \cdots & x_1^{r-1} \\ \mathbf{1}_k & \vdots & \\ x_k & \cdots & x_k^{r-1} \end{pmatrix},$$
$$\mathbf{y} = \begin{pmatrix} y_{11} \\ y_{12} \\ \vdots \\ y_{kn_k} \end{pmatrix}, \qquad \boldsymbol{\theta} = \begin{pmatrix} \theta_1 \\ \theta_2 \\ \vdots \\ \theta_r \end{pmatrix}, \qquad \boldsymbol{\mu} = \begin{pmatrix} \mu(x_1) \\ \vdots \\ \mu(x_k) \end{pmatrix}.$$

Then,  $E(y) = L\mu$  and  $H_0$  in (2.2) can be represented as

$$H_0: \mathcal{E}(y) = LX\theta. \tag{2.4}$$

Since L is full rank, the testing problem is the same problem of testing

$$\tilde{H}_0: (I_k - X(X'X)^{-1}X')\mu = \mathbf{0}$$
(2.5)

under the linear model,

$$y = L\mu + \mathscr{E}$$
 where  $\mathscr{E} = (\varepsilon_{11}, \dots, \varepsilon_{1n_1}, \dots, \varepsilon_{k1}, \dots, \varepsilon_{kn_k})'$ . (2.6)

Noting that  $\Pi_X^{\perp} = I_k - X(X'X)^{-1}X$  is a projection matrix of rank k - r, let H' be  $k \times (k - r)$  orthonormal matrix whose columns are the eigenvectors corresponding to the eigenvalue 0 of  $\Pi_X^{\perp}$ . Then  $\Pi_X^{\perp} = H'H$ , and (2.4) is equivalent to  $H\mu = 0$ .

Let

$$\hat{\boldsymbol{\mu}} = (L'L)^{-1}L'\boldsymbol{y}, \qquad S_h = \hat{\boldsymbol{\mu}}'H'\{H(L'L)^{-1}H'\}^{-1}H\hat{\boldsymbol{\mu}},$$

$$S_e = \boldsymbol{y}'(I_n - \Pi_L)\boldsymbol{y} \qquad \text{where } \Pi_L = L(L'L)^{-1}L'.$$
(2.7)

Then, the likelihood ratio test under normality rejects the null hypothesis of (2.5) for large values of

$$\frac{S_h/(k-r)}{S_e/(n-k)}. (2.8)$$

Let

$$\Pi_{LX} = LX(X'L'LX)^{1}X'L', 
\Pi_{LH} = L(L'L)^{-1}H'\{H(H(L'L)^{-1}H'\}^{-1}H(L'L)^{-1}L'.$$
(2.9)

Then  $\Pi_L = \Pi_{LX} + \Pi_{LH}$  and  $S_h = y' \Pi_{LH} y$ , which shows that (2.8) is the same as the test statistic (2.3).

## 3. Asymptotic expansion

In this section, we give the asymptotic expansion of null distribution of T under nonnormality when k is fixed and  $n \to \infty$ .

Set

$$Z = (L'L)^{-1/2}L'\mathscr{E}, \qquad U = Z(n^{-1}S_e)^{-1/2}.$$
 (3.1)

Then, under the null hypothesis, T can be expanded as

$$(k-r)T = U'\Omega U - \frac{k}{n}U'\Omega U + O_p(n^{-3/2}),$$
 (3.2)

where

$$\Omega = (L'L)^{-1/2}H'\{H(L'L)^{-1}H'\}^{-1}H(L'L)^{-1/2}.$$

This is the same form as  $T_G$  in [4] (page 19) with p = 1,  $r_1 = r_2 = 0$ . Hence we can apply the results of them to our problem. The coefficients of the asymptotic expansion depend on

$$a_{1} = \frac{1}{8} \{ n \text{ tr } D_{\Psi}^{2} - (k - r)((k - r) + 2) \}, \qquad a_{2} = \frac{n}{12} \mathbf{1}'_{n} \Psi_{(3)} \mathbf{1}_{n},$$

$$a_{3} = \frac{n}{8} \mathbf{1}'_{n} D_{\Psi} \Psi D_{\Psi} \mathbf{1}_{n}, \qquad a_{4} = \frac{1}{12} \mathbf{1}'_{n} D_{\Psi} \Psi \mathbf{1}_{n}, \qquad a_{5} = \frac{1}{8n} \mathbf{1}'_{n} \Psi \mathbf{1}_{n},$$

where

$$\Psi = (\psi_{ab}) = \Pi_{LH} : n \times n,$$

$$D_{\Psi} = \operatorname{diag}(\psi_{11}, \dots, \psi_{nn}), \qquad \Psi_{(3)} : (a, b) \text{th element is } \psi_{ab}^{3}.$$

Since  $\Psi = \Pi_{LH} = \Pi_L - \Pi_{LX}$  and both L and LH include  $\mathbf{1}_n$  as the first column, it follows that  $a_4 = a_5 = 0$ . Therefore the coefficients of the asymptotic expansion of the distribution of T can be simplified as follows.

THEOREM 3.1. Assume that

A1. For any 
$$j$$
,  $\frac{n}{n_i} = O(1)$ ,

B1. 
$$E(|\varepsilon|^8) < \infty$$
, and

B2. Cramér condition for the joint distribution of  $\varepsilon$  and  $\varepsilon^2$  is hold, that is, for any b > 0,  $\sup_{|t_1|+|t_2|>b} |\mathrm{E}[\exp(it_1\varepsilon+it_2\varepsilon^2)]| < 1$ .

Then the null distribution of T is expanded as

$$P[(k-r)T \le x] = G_{k-r}(x) + \frac{1}{n} \sum_{i=0}^{3} b_j G_{k-r+2j}(x) + o(n^{-1}),$$
 (3.3)

where

$$b_0 = -\kappa_3^2(a_2 + a_3) + \kappa_4 a_1 + \frac{1}{4}(k - r)(k - r - 2),$$

$$b_1 = 3\kappa_3^2(a_2 + a_3) - 2\kappa_4 a_1 - \frac{1}{2}(k - r)^2,$$

$$b_2 = -3\kappa_3^2(a_2 + a_3) + \kappa_4 a_1 + \frac{1}{4}(k - r)((k - r) + 2),$$

$$b_3 = \kappa_3^2(a_2 + a_3).$$

The equation (3.3) is also represented as

$$P[T \le x] = G_{k-r}(x) + \frac{2x}{n(k-r)} g_{k-r}(x)$$

$$\times \left\{ b_1 + b_2 + b_3 + \frac{(b_2 + b_3)x}{k - r + 2} + \frac{b_3 x^2}{(k - r + 2)(k - r + 4)} \right\}$$

$$+ o(n^{-1}), \tag{3.4}$$

which can be used to derive the Cornish Fisher expansion of the percent points.

The proof of the validity of the asymptotic expansion by use of the Cramér condition is given in [2], and for general methods for deriving asymptotic expansions and the Cornish Fisher expansions, the reader is refered to [1].

## 4. Robustness against nonnormality

Using (3.4), we can expand the expectation of T as

$$E(T) = \left(1 + \frac{c_1}{n}\right) + o(n^{-1}),\tag{4.1}$$

where

$$c_1 = \frac{2}{k-r} \sum_{j=1}^{3} jb_j = \frac{2}{k-r}.$$

Therefore, the expectation of T under nonnormality is equal to the one under normality, up to  $o(n^{-1})$ .

While the variance of T can be expanded as

$$E(T^{2}) = \frac{k - r + 2}{k - r} \left( 1 + \frac{c_{2}}{n} \right) + o(n^{-1}), \tag{4.2}$$

where

$$c_2 = \frac{4}{(k-r)(k-r+2)} \{ (k-r+2)(b_1+2b_2+3b_3) + 2(b_2+3b_3) \}$$
$$= \frac{8}{(k-r)(k-r+2)} \left\{ a_1 \kappa_4 + \frac{1}{4}(k-r)(k-r+2) \right\}.$$

If  $a_1 = 0$ , the variance of T under nonnormality is also equal to the one under normality, and we can say that the Lack-of-Fit test is robust against the nonnormality. Suppose that  $n_1 = \cdots = n_k = m$ . Then

$$a_1 = \frac{1}{8} \{ n \text{ tr } D_{\Psi}^2 - (k - r)(k - r + 2) \}$$
$$= \frac{1}{8} \left( k \frac{\sum_{j=1}^k (x_j - \bar{x})^4}{\left(\sum_{j=1}^k (x_j - \bar{x})^2\right)^2} + 3 - 2k \right).$$

Therefore, when  $a_1 = 0$ ,

$$\frac{\sum_{j=1}^{k} (x_j - \bar{x})^4}{\left(\sum_{j=1}^{k} (x_j - \bar{x})^2\right)^2} = 2 - 3/k.$$

However, when  $k \ge 3$ , the maximum value of the left-hand side is smaller than the right-hand side. Hence  $a_1 = 0$  cannot be hold. We have to be careful about the kurtosis when we use the Lack-of-Fit test for nonnormal data.

#### 5. Simulation

We make a simulation in case of simple linear regression analysis based on the previous results.

#### 5.1. Methods

The simulation method is as follows. First, we estimate the percent point of test statistic T using Monte-Carlo method. Then, we compare it with percent point calculated by the asymptotic expansion (3.3).

In order to calculate the approximation of percent point, we use the Cornish-Fisher expansion. Let t(v) and v be the right percent point and the percent point of limit distribution of T, respectively. Then,

$$P[T \cdot (k-r) \ge t(v)] = P(\chi_{k-r}^2 \ge v),$$

where  $\chi^2_{k-r}$  is the random variable of  $\chi^2$ -distribution with k-r degrees of freedom. From (3.4), t(v) has the expression

$$t(u) = \frac{u}{k-r} + \frac{2u}{n(k-r)^2} \left\{ b_1 + b_2 + b_3 + \frac{(b_2 + b_3)u}{(k-r+2)(k-r)} + \frac{b_3 u^2}{(k-r+2)(k-r+4)(k-r)^2} \right\} + o(n^{-1}).$$
(5.1)

In (5.1), there exists unknown parameters  $\kappa_3$  and  $\kappa_4$ . So, we replace them with their estimators

$$\hat{\kappa}_3 = \frac{n}{(n-1)(n-2)} \sum_{j=1}^n \tilde{\varepsilon}_j^3, \qquad \hat{\kappa}_4 = \frac{n(n+1)}{(n-1)(n-2)(n-3)} \sum_{j=1}^n \tilde{\varepsilon}_j^4 - 3,$$

where

$$\tilde{\varepsilon}_j = \hat{\sigma}^{-1}(\varepsilon_j - \overline{\varepsilon}), \qquad \overline{\varepsilon} = \frac{1}{n} \sum_{i=1}^n \varepsilon_j, \qquad \hat{\sigma}^2 = \frac{1}{n-1} \sum_{i=1}^n (\varepsilon_j - \overline{\varepsilon})^2.$$

The distributions considered are the followings:

- · The standard normal distribution;
- Uniform distribution on  $(-\sqrt{3}, \sqrt{3})$ ;
- Exponential distribution with the mean 1; and
- t-distribution with 5 degrees of freedom.

In the case of simple linear regression analysis, parameter r is r = 2. We assume that k = 4. Then, H defined before (2.7) can be calculated numer-

ically. The data of explanatory variables x and sample sizes  $n = (n_1, \dots, n_4)'$  of each response variables are shown, respectively, as

$$x$$
: (1)  $(1,2,3,4)'$ , (2)  $(1,3,5,7)'$ , (3)  $(1,2,7,8)'$ ,

$$(4) (1,6,7,8)', (5) (1,2,3,8)', (6) (-2,-1,1,2)',$$

$$n:$$
  $(8,8,8,8)',$   $(56,8,8,56)'.$ 

## 5.2. Results and comments

Table 1 and Table 2 give the actual test sizes for the nominal 10%, 5% and 1% test in several cases of n and x. For each row in Tables, top and second

Table 1.	The resu	lts of	simulation	when	n =	(8, 8, 8, 8)	′
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	Normal Nominal Sizes			Uniform Nominal Sizes			Exponent Nominal Sizes			<i>t</i> -distribution Nominal Sizes		
x	10%	5%	1%	10%	5%	1%	10%	5%	1%	10%	5%	1%
(1)	10.34	5.26	0.96	9.58	4.70	0.84	9.17	4.87	0.78	9.65	4.11	0.68
	10.28	5.25	0.96	9.53	4.70	0.84	9.05	4.87	0.78	9.57	4.11	0.68
	10.71	5.43	1.01	9.31	4.61	0.84	11.39	6.08	1.07	11.68	5.13	0.92
	10.69	5.42	1.01	9.23	4.55	0.84	11.43	6.10	1.07	11.73	5.17	0.92
(2)	10.34	5.26	0.96	9.91	5.30	1.04	9.29	4.44	0.98	8.88	4.76	0.64
	10.28	5.25	0.96	9.87	5.29	1.04	9.29	4.44	0.98	8.88	4.76	0.64
	10.71	5.43	1.01	9.83	5.20	1.04	12.36	5.75	1.11	10.77	5.66	0.89
	10.69	5.42	1.01	11.26	6.16	0.84	12.51	5.78	1.11	10.78	5.66	0.89
(3)	10.37	5.27	1.11	9.37	4.33	1.02	9.90	4.98	0.80	9.35	4.38	0.72
	10.31	5.25	1.11	9.34	4.33	1.02	9.89	4.98	0.80	9.35	4.38	0.72
	10.87	5.46	1.15	9.27	4.26	1.02	11.91	5.93	1.09	11.99	5.82	1.04
	10.87	5.46	1.15	9.24	4.26	1.02	12.05	5.93	1.09	11.99	5.82	1.04
(4)	10.47	5.38	1.03	9.82	4.70	0.84	9.89	4.85	0.98	9.85	4.56	1.01
	10.46	5.37	1.03	9.79	4.70	0.82	9.75	4.85	0.98	9.85	4.56	1.01
	10.68	5.56	1.04	9.75	4.70	0.82	12.19	6.27	1.21	11.45	4.97	1.18
	10.67	5.56	1.04	9.69	4.70	0.82	12.23	6.39	1.21	11.46	4.97	1.18
(5)	10.27	5.17	1.03	9.51	4.50	0.78	9.81	5.00	0.72	10.25	5.56	1.24
	10.20	5.16	1.03	9.51	4.44	0.78	9.78	5.00	0.72	10.22	5.56	1.24
	10.56	5.26	1.07	9.47	4.41	0.78	12.39	6.38	1.24	11.79	6.30	1.59
	10.56	5.26	1.07	9.47	4.41	0.78	12.43	6.48	1.24	11.79	6.30	1.59
(6)	10.30	5.17	0.98	10.54	5.32	1.14	9.68	4.69	0.87	9.95	5.03	0.73
	10.24	5.16	0.98	10.53	5.32	1.14	9.60	4.69	0.87	9.87	4.99	0.73
	10.60	5.42	1.03	10.46	5.24	1.12	11.67	6.19	1.21	11.70	5.91	0.98
	10.59	5.42	1.03	10.46	5.21	1.12	11.71	6.20	1.21	11.82	5.91	0.98

	Normal Nominal Sizes			Uniform Nominal Sizes			Exponent Nominal Sizes			<i>t</i> -distribution Nominal Sizes		
x	10%	5%	1%	10%	5%	1%	10%	5%	1%	10%	5%	1%
(1)	10.37	5.18	0.99	9.72	5.22	0.95	9.82	4.76	1.03	11.33	5.96	1.07
	10.37	5.17	0.99	9.72	5.22	0.95	9.82	4.76	1.03	11.33	5.94	1.07
	9.82	4.85	0.95	10.15	5.35	0.97	19.08	9.88	2.04	7.27	3.83	0.62
	9.79	4.84	0.95	10.15	5.36	0.97	19.71	10.10	2.04	7.12	3.81	0.62
(2)	10.37	5.18	0.99	10.20	5.21	1.08	9.20	4.36	1.04	10.81	5.53	1.01
	10.36	5.17	0.99	10.20	5.21	1.08	9.18	4.36	1.04	10.81	5.53	1.01
	9.82	4.85	0.95	10.34	5.27	1.10	18.02	9.24	1.91	7.03	3.39	0.51
	9.79	4.84	0.95	10.34	5.27	1.10	18.68	9.28	1.91	7.02	3.36	0.50
(3)	10.37	5.27	0.87	9.77	5.26	1.15	9.44	4.53	0.90	11.06	5.38	0.87
	10.36	5.27	0.87	9.76	5.26	1.15	9.42	4.53	0.90	11.00	5.38	0.87
	9.83	4.94	0.82	9.94	5.42	1.17	17.32	8.83	1.68	7.52	3.36	0.58
	9.82	4.94	0.82	9.94	5.42	1.17	17.69	8.95	1.68	7.45	3.29	0.59
(4)	10.41	5.27	1.00	9.52	4.47	0.73	9.73	4.70	1.06	10.03	4.64	0.83
	10.39	5.27	1.00	9.52	4.47	0.73	9.72	4.70	1.06	10.03	4.64	0.83
	9.84	4.91	0.98	9.80	4.62	0.73	18.53	9.83	2.01	5.99	2.66	0.51
	9.83	4.91	0.98	9.80	4.63	0.73	18.96	9.97	2.02	5.79	2.60	0.51
(5)	10.25	5.05	0.91	9.38	4.89	0.73	9.79	5.00	0.95	10.94	5.47	1.07
	10.24	5.05	0.91	9.35	4.89	0.73	9.79	5.00	0.95	10.94	5.46	1.07
	9.73	4.71	0.86	9.62	5.03	0.74	19.22	9.93	2.12	6.74	3.36	0.71
	9.71	4.71	0.86	9.62	5.03	0.74	19.67	10.09	2.12	6.61	3.35	0.71
(6)	10.37	5.13	1.00	9.76	4.72	1.00	9.96	4.57	0.82	10.69	5.38	1.07
	10.36	5.13	1.00	9.76	4.72	1.00	9.96	4.57	0.82	10.66	5.38	1.07
	9.78	4.86	0.96	9.99	4.78	1.01	18.71	9.95	2.04	6.93	3.09	0.70
	9.76	4.85	0.96	9.99	4.78	1.01	19.24	10.12	2.05	6.72	3.10	0.70

Table 2. The results of simulation when n = (56, 8, 8, 56)'

stairs express the actual test sizes based on F-distribution and limit distribution of (3.4), the third and bottom stairs show the actual sizes by using t(v) and  $\hat{t}(v)$ , respectively.

In the Tables, it is shown that there are good approximation by use of (3.4) when sample sizes are balanced. However, when sample sizes are unbalanced, approximations are not very good.

In addition, using the previous results, we calculate the approximate expectations and show the results in Table 3. For each row in Table 3, the top stairs express the actual expectation, second stairs express the approximate expectation, and bottom stairs show the approximate expectation by estimated parameters. Note that the expectation of F-distribution with k-r and n-k

		n = (8,	8, 8, 8)		n = (56, 8, 8, 56)					
	Normal	Uniform	Exponent	<i>t</i> -dist.	Normal	Uniform	Exponent	<i>t</i> -dist.		
(1)	1.0237	1.0013	1.0910	1.0789	1.0712	0.9598	1.0792	1.0327		
	0.9375	0.9375	0.8433	0.9375	0.9375	0.9375	0.9058	0.9375		
	0.9375	0.9375	0.9374	0.9375	0.9375	0.9375	0.9375	0.9375		
(2)	1.0107	1.1457	1.0731	1.0184	1.0579	1.0087	1.0149	1.0115		
	0.9375	0.9375	0.8433	0.9375	0.9375	0.9375	0.9058	0.9375		
	0.9375	0.9375	0.9374	0.9375	0.9375	0.9375	0.9375	0.9375		
(3)	0.9696	0.9030	1.0210	1.1358	0.9721	1.0282	1.0341	1.0125		
	0.9375	0.9375	0.8643	0.9375	0.9375	0.9375	0.9087	0.9375		
	0.9375	0.9375	0.9374	0.9375	0.9375	0.9375	0.9376	0.9375		
(4)	0.8780	1.0979	1.2321	1.0693	1.0478	0.9986	0.9975	1.0296		
	0.9375	0.9375	0.8278	0.9375	0.9375	0.9375	0.9029	0.9375		
	0.9375	0.9375	0.9373	0.9375	0.9375	0.9375	0.9375	0.9375		
(5)	1.0032	1.0042	1.0610	1.0274	0.9970	1.0095	1.0033	1.0346		
	0.9375	0.9375	0.8446	0.9375	0.9375	0.9375	0.9047	0.9375		
	0.9375	0.9375	0.9374	0.9375	0.9375	0.9375	0.9375	0.9375		
(6)	1.0595	0.9506	1.3707	1.1213	1.0431	0.9922	1.0806	0.9840		
	0.9375	0.9375	0.8492	0.9375	0.9375	0.9375	0.9063	0.9375		
	0.9375	0.9375	0.9374	0.9375	0.9375	0.9375	0.9375	0.9375		

Table 3. The results of simulation of expectation.

degrees of freedom is (n-k)/(n-k-2). It is seen that each expectation has similar value in each distribution except for the case of exponential distribution. In the case of exponential distribution, there were some differences between the true values and approximated values of the expectations, which suggests that the skewness may affect to the expectation in higher order expansions.

### 6. Problems in the future

In this paper, we consider an asymptotic approximation of null-distribution for Lack-of-Fit statistics when the number of explanatory variables k is fixed. We derive the form of asymptotic expansion in the case of 1-dimension response variables. In addition, we consider robustness of the test against nonnormality. In the future, we want to consider the methods of obtaining good approximation when sample sizes are unbalanced, and the application of these results.

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