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Fiducial generalized *p*-values for testing zero-variance components in linear mixed-effects models

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Abstract Linear mixed-effects models are widely used in analysis of longitudinal data. However, testing for zero-variance components of random effects has not been well-resolved in statistical literature, although some likelihood-based procedures have been proposed and studied. In this article, we propose a generalized p-value based method in coupling with fiducial inference to tackle this problem. The proposed method is also applied to test linearity of the nonparametric functions in additive models. We provide theoretical justifications and develop an implementation algorithm for the proposed method. We evaluate its finite-sample performance and compare it with that of the restricted likelihood ratio test via simulation experiments. We illustrate the proposed approach using an application from a nutritional study.

Keywords fiducial distribution, generalized pivotal quantity, generalized test variable, penalized spline additive models, restricted likelihood ratio test, structural equation, zero-variance components

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1 Introduction

A powerful tool for analysis of longitudinal data is linear mixed-effects (LME) models, in which within-subject and between-subject variations are both considered. Likelihood-based estimation and inference for the population parameters of the LME models (see [20]) have been well-studied in statistical literature. Inference procedures for LME models are implemented in well-developed statistical software packages such as SAS and Splus/R with wide applications in many scientific fields (see [9, 23, 32, 33]). However, efforts in statistical inference for the variance of random effects seem to be incommensurable although the initial attempt can be traced back to [34]. Mixed-effects analysis of variance (ANOVA) models have been mostly studied to test the variance of random effects (see [18]). Even in the simple ANOVA models, to find an optimal test for the variance of the random effects is far more complicated when the data are unbalanced, since the partition of total sum of squares is not unique and the sums of squares in an ANOVA model are generally not independent. In consequence, no exact or optimal test for the variance

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of the random effects in ANOVA models with unbalanced data is available. For this reason, the main research effort has been shifted to derive proper tests, which may not be optimal in general sense but have some good frequentist properties (see [23]). For example, Das and Sinha [7] derived a locally best invariant test.

In testing variance components of random effects, a challenging problem is how to test zero variance, since the null hypothesis of the variance parameter falls on the boundary of the parameter space in this case. This testing problem is not standard. Self and Liang [26] developed an asymptotic likelihood ratio test under this nonstandard situation for *independent* data. Stram and Lee [28] applied Self and Liang's theory to variance-components testing in LME models for longitudinal data. They found that the finite-sample distribution of the test statistics could be approximated by a $0.5\mathcal{X}_0^2 + 0.5\mathcal{X}_1^2$ mixture. However, the $0.5\mathcal{X}_0^2 + 0.5\mathcal{X}_1^2$ mixture approximation can be far inaccurate, which has been noticed by [23, 27], and recently confirmed by a series of papers [3–6]. These recent articles derived asymptotic distributions of the probability mass at zero of the log (residual) likelihood ratio statistics and numerically analyzed why the $0.5\mathcal{X}_0^2 + 0.5\mathcal{X}_1^2$ mixture can be a rather poor approximation. Crainiceanu and Ruppert [3, 4] and Crainiceanu et al. [6] proposed a simulation-based approach to deal with this problem. Their asymptotic distribution is a maximizer of a stochastic process, which needs to be evaluated via Monte Carlo simulations, and thus their method is computationally expensive. They pointed out that their methods are only applicable to the models with a single variance component. More recently, Greven et al. [13] made further efforts to avoid the simulation approach proposed by [4, 5] and proposed two approximation methods for the finite sample distribution of the likelihood ratio statistics. Although the asymptotic distribution of the restricted likelihood ratio (RLR) test is derived for a single variance component for the case of LME models, the extension to multiple variance components remains challenging. In addition, the proposed RLR test could not maintain the stated level of type I error even for moderate sample sizes, and its type I error is generally higher than the nominal level (see [25]). Thus, to develop a zero-variance test and a corresponding efficient implementation procedure under the conventional concept of likelihood-based methods is needed.

Tsui and Weerahandi [31] proposed an alternative generalized p-value for hypothesis testing with an emphasis on the exact probability theory instead of asymptotic approximations. The idea was originally developed to solve the hypothesis testing problem such as Behrens-Fisher problem in the presence of nuisance parameters. Weerahandi [35] extended the idea for variance component testing in balanced one-way or two-way mixed models. Zhou and Mathew [38] further extended it to a balanced ANOVA model when an exact F-test does not exist. They also applied generalized p-values for comparing variance components in two dependent unbalanced mixed models as well as in two dependent balanced mixed models. Arendacká [1] applied the method by [38], and constructed generalized confidence intervals on the variance component in mixed linear models with two variance components. Weerahandi [37] provided a comprehensive survey on the generalized p-value methods with various applications. Tian [29, 30] applied generalized p-values for several statistical inference problems. One of the appealing features of the generalized p-value approach is that it can provide an exact solution for the hypothesis testing problem where the classic approaches are not applicable. However, the generalized p-value is not easy to construct, even for the simple Behrens-Fisher problem [31]. Weerahandi [37] proposed a substitution method. The key step of his method is to express the parameters of interest as a function of a statistic and a random variable with its distribution free of unknown parameters. But no general rule was given on how to construct such a function and no theoretical justification was provided for the approach.

Fisher [12] proposed a concept of the fiducial inference as an alternative to the traditional hypothesis testing. Weerahandi [36] indicated that the generalized p-value approach is also in the spirit of fiducial inference. The fiducial distribution of the parameters is based on the observed data only, and does not involve any prior distributions compared to the Bayesian inference. More details for derivation of fiducial distributions can be found in [8]. Recently, Hannig [14] and Hannig et al. [16] combined Fisher's fiducial arguments and the generalized p-value approach and developed a fiducial recipe for generalized confidence intervals. Hannig et al. [16] proposed fiducial generalized confidence intervals for variance components in an unbalanced two-variance component mixed model. But as pointed out in [15], their fiducial interval is conservative when the ratio of the variance of random-effects over the variance of the error is less than 1. In addition, their method is limited to the two-variance component mixed model since a closed-form for the minimum sufficient statistics is needed.

In this paper, we develop a fiducial generalized p-value-based method, which is different from [14–16], to derive the generalized fiducial distributions which is easier to assess compared with the calculation of the conditional probability of the generalized fiducial intervals, since the later requires solving several integral equations. Compared with the existing methods, our proposed method has several advantages: (i) We provide a general recipe to derive the tests for zero-variance components. In addition, we theoretically justify that our tests work properly although they may not be optimal in a conventional sense. (ii) The implementation algorithms can be easily developed for the proposed methods and are computationally expedient. (iii) Numerical studies demonstrate that the proposed method is promising and better than the existing methods under different situations. (iv) The proposed method can be applied to test the linearity in nonparametrically additive models.

The outline of the paper is as follows. Section 2 gives a general recipe of the proposed fiducial generalized p-value method and present the main results. Section 3 introduces the linear mixed-effects models (LME) and the restricted likelihood ratio test, and uses the proposed general recipe to derive the test for zero-variance components LME. Section 4 applies the proposed method for checking linearity in additive models. Section 5 presents the simulation results to compare the proposed method with the existing methods, and Section 6 analyzes a dataset from a nutritional study using the proposed tests. Discussions and conclusions are given in Section 7. Some technical details are located in Appendices A and B.

2 A general recipe of fiducial generalized *p*-values

Let $\boldsymbol{\Xi}$ be a random vector with a probability distribution $\mathbf{P}_\eta(\cdot)$, where η is an unknown vector, and $\theta = \theta(\eta) \in \Theta = [\theta_1, \theta_2]$ is a parameter of interest. θ_1 may be $-\infty$, and θ_2 may be ∞. An observation of $\boldsymbol{\Xi}$ is denoted by $\boldsymbol{\xi}$. We are interested in the one-sided hypothesis: $H_0 : \theta \leqslant \theta_0 \leftrightarrow H_1 : \theta > \theta_0$. Tsui and Weerahandi [31] introduced the concept of generalized inference for hypothesis testing. See [37] for a detailed discussion on how to derive a generalized p-value. Assume that the test variable $\boldsymbol{R} = \boldsymbol{R}(\boldsymbol{\Xi}; \boldsymbol{\xi}, \eta)$ is a function of $\boldsymbol{\Xi}$, the observed value $\boldsymbol{\xi}$ and the parameters $\eta = (\theta, \delta)$. $\boldsymbol{R}$ is said to be a generalized test variable if the following three properties hold:

(i) the observation $\boldsymbol{r} = \boldsymbol{R}(\boldsymbol{\xi}; \boldsymbol{\xi}, \eta)$ is free of nuisance parameters δ;

(ii) $\boldsymbol{R}$ has a probability distribution free of unknown parameters; and

(iii) $\boldsymbol{R} = \boldsymbol{R}(\boldsymbol{\Xi}; \boldsymbol{\xi}, \eta)$ is stochastically increasing in θ, i.e., $\mathrm{P}\{\boldsymbol{R}(\boldsymbol{\Xi}; \boldsymbol{\xi}, \eta) \geqslant \boldsymbol{r}\}$ is nondecreasing in θ.

A large observed value of $\boldsymbol{R}$ suggests an evidence against null hypothesis H_0, and the generalized p-value is given by

$$p = \sup_{\theta \leqslant \theta_0} \mathrm{P}(\boldsymbol{R} \geqslant \boldsymbol{r} \,|\, \theta) = \mathrm{P}(\boldsymbol{R} \geqslant \boldsymbol{r} \,|\, \theta = \theta_0).$$

A small p-value indicates that we cannot accept the null hypothesis H_0.

Weerahandi [37] proposed a substitution method to derive the test. The key step of his method is to express the parameter of interest θ as a function of random vector $\boldsymbol{\Xi}$ and a random variable $\boldsymbol{U}$ with its distribution free of the unknown parameters. This manipulation is, however, not easy to implement, and difficult, if not impossible, to justify. Here, we propose to use the concept of fiducial inference to construct the generalized p-value, which stems from the definition of fiducial distributions given by [8]. Hannig et al. [16] proposed a general method for constructing fiducial generalized confidence interval based on structural equation. In the following, we give a general method for fiducial generalized p-value based on structural equation. Suppose that we have a structural equation which can be expressed as

$$\boldsymbol{\Xi} = \boldsymbol{G}(\eta, \boldsymbol{U})$$

for a random variable $\boldsymbol{U}$, whose distribution is known. The equation $\boldsymbol{\xi} = \boldsymbol{G}(\eta, \boldsymbol{u})$ has a unique solution for η, say $\boldsymbol{G}^{-1}(\boldsymbol{\xi}, \boldsymbol{u})$. Then the distribution of $\boldsymbol{G}^{-1}(\boldsymbol{\xi}, \boldsymbol{U})$ and $\theta(\boldsymbol{G}^{-1}(\boldsymbol{\xi}, \boldsymbol{U}))$ are the fiducial distributions of η and $\theta(\eta)$ with respect to observed $\boldsymbol{\xi}$, respectively.

Remark 2.1. Although $\theta \in \Theta = [\theta_1, \theta_2]$ does not mean that $\theta(\boldsymbol{G}^{-1}(\boldsymbol{\xi}, \boldsymbol{u}))$ is always in Θ for all $\boldsymbol{\xi}$ and $\boldsymbol{u}$, a minor modification can easily remedy this problem, i.e., let $\theta^*(\boldsymbol{G}^{-1}(\boldsymbol{\xi}, \boldsymbol{u})) = \theta_1 \boldsymbol{I}_{\{\theta(\boldsymbol{G}^{-1}(\boldsymbol{\xi},\boldsymbol{u}))<\theta_1\}} + \theta(\boldsymbol{G}^{-1}(\boldsymbol{\xi}, \boldsymbol{u}))\boldsymbol{I}_{\{\theta_1 \leqslant \theta(\boldsymbol{G}^{-1}(\boldsymbol{\xi},\boldsymbol{u}))<\theta_2\}} + \theta_2 \boldsymbol{I}_{\{\theta(\boldsymbol{G}^{-1}(\boldsymbol{\xi},\boldsymbol{u}))\geqslant\theta_2\}}$. Note that

$$\begin{aligned}\{\boldsymbol{U} : \theta^*(\boldsymbol{G}^{-1}(\boldsymbol{\xi}, \boldsymbol{U})) \leqslant \theta\} &= \{\boldsymbol{U} : \theta(\boldsymbol{G}^{-1}(\boldsymbol{\xi}, \boldsymbol{U})) \leqslant \theta_1\} \cup \{\boldsymbol{U} : \theta_1 \leqslant \theta(\boldsymbol{G}^{-1}(\boldsymbol{\xi}, \boldsymbol{U})) \leqslant \theta\} \\ &= \{\boldsymbol{U} : \theta(\boldsymbol{G}^{-1}(\boldsymbol{\xi}, \boldsymbol{U})) \leqslant \theta\}.\end{aligned}$$

Therefore, the distributions of $\theta(\boldsymbol{G}^{-1}(\boldsymbol{\xi}, \boldsymbol{U}))$ and $\theta^*(\boldsymbol{G}^{-1}(\boldsymbol{\xi}, \boldsymbol{U}))$ are the same.

The following theorem provides a general guidance for how to obtain a generalized p-value through a structural equation. Its proof is not difficult, but this connection to fiducial inference theory is novel and critical for us to establish a test for zero-variance components.

Theorem 2.2. *Assume that the equation $\boldsymbol{\xi} = \boldsymbol{G}(\eta, \boldsymbol{u})$ has a unique solution for η, denoted by $\boldsymbol{G}^{-1}(\boldsymbol{\xi}, \boldsymbol{u})$, and the equation also has a unique solution for any $\boldsymbol{u}$, denoted by $\boldsymbol{u} = \boldsymbol{H}(\boldsymbol{\xi}, \eta)$. Then $\boldsymbol{R}(\Xi; \boldsymbol{\xi}, \eta) = \theta^*(\boldsymbol{G}^{-1}(\boldsymbol{\xi}, \boldsymbol{H}(\Xi, \eta))) - \theta$ is a generalized test variable.*

Proof. It suffices to verify that $\boldsymbol{R}(\Xi; \boldsymbol{\xi}, \eta)$ satisfies the three properties. Note that

$$\boldsymbol{R}(\boldsymbol{\xi}; \boldsymbol{\xi}, \eta) = \theta^*(\boldsymbol{G}^{-1}(\boldsymbol{\xi}, \boldsymbol{H}(\boldsymbol{\xi}, \eta))) - \theta = \theta^*(\boldsymbol{G}^{-1}(\boldsymbol{\xi}, \boldsymbol{u})) - \theta = \theta(\eta) - \theta = 0.$$

Property (i) holds. Furthermore, $\theta^*(\boldsymbol{G}^{-1}(\boldsymbol{\xi}, \boldsymbol{H}(\Xi, \eta))) = \theta^*(\boldsymbol{G}^{-1}(\boldsymbol{\xi}, \boldsymbol{U}))$ is free of any other parameters, and the distribution of $\boldsymbol{R}(\Xi; \boldsymbol{\xi}, \eta) = \theta^*(\boldsymbol{G}^{-1}(\boldsymbol{\xi}, \boldsymbol{U})) - \theta$ dose not depend on other parameters. In addition, we have

$$\mathrm{P}(\boldsymbol{R}(\Xi; \boldsymbol{\xi}, \eta) \geqslant \boldsymbol{R}(\boldsymbol{\xi}; \boldsymbol{\xi}, \eta)) = \mathrm{P}(\theta^*(\boldsymbol{G}^{-1}(\boldsymbol{\xi}, \boldsymbol{U})) \geqslant \theta) = \mathrm{P}(\theta(\boldsymbol{G}^{-1}(\boldsymbol{\xi}, \boldsymbol{U})) \geqslant \theta),$$

which is nonincreasing in θ. The proof is completed. □

We call the value, $p = \mathrm{P}(\theta(\boldsymbol{G}^{-1}(\boldsymbol{\xi}, \boldsymbol{U})) \leqslant \theta_0)$, as the fiducial generalized p-value.

3 Zero-variance component test

3.1 LME

Consider the LME model

$$\boldsymbol{y}_i = \boldsymbol{X}_i \boldsymbol{\beta} + \boldsymbol{Z}_i \boldsymbol{b}_i + \boldsymbol{\varepsilon}_i, \quad i = 1, \ldots, n,$$

where $\boldsymbol{\beta}$ is a $p \times 1$ vector of fixed regression coefficients, $\boldsymbol{b}_i$ is a $k \times 1$ vector of random coefficients specific to the subject i and $\boldsymbol{b}_i \sim N(0, \boldsymbol{D})$. $\boldsymbol{y}_i = (y_{i1}, \ldots, y_{im_i})'$ denotes the response variables, $\boldsymbol{X}_i(m_i \times p)$, and $\boldsymbol{Z}_i(m_i \times k)$ represents the known covariate matrices for the fixed and random effects (assuming full column rank) for the i-th subject, and $\boldsymbol{\varepsilon}_i \sim N(0, \boldsymbol{R}_i)$ is an error vector being independent of $\boldsymbol{b}_i$. Both the covariance matrices $\boldsymbol{D}$ and $\boldsymbol{R}_i$ may have special structures, and in this paper we assume that $\boldsymbol{R}_i = \sigma_\varepsilon^2 \boldsymbol{I}_{m_i}$, where σ_ε^2 is an unknown parameter and $\boldsymbol{I}_{m_i}$ is an $m_i \times m_i$ identity matrix. Let $N = \sum_{i=1}^n m_i$ be the total number of observations, and $\boldsymbol{\theta}$ be the vector of parameters in the model, including $\boldsymbol{\beta}$, σ_ε^2 and the parameters in $\boldsymbol{D}$. The above LME model can be written as

$$\boldsymbol{Y} = \boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{Z}\boldsymbol{b} + \varepsilon, \quad \boldsymbol{b} \sim N(0, \boldsymbol{G}), \tag{3.1}$$

where $\boldsymbol{y}$ is an $N \times 1$ vector of observations, $\boldsymbol{X} = (\boldsymbol{X}_1', \ldots, \boldsymbol{X}_n')'$ is an $N \times p$ matrix of rank p, $\boldsymbol{Z} = \mathrm{diag}(\boldsymbol{Z}_1, \ldots, \boldsymbol{Z}_n)$ is an $N \times r$ block-diagonal matrix of rank $r = nk$, $\boldsymbol{b} = (\boldsymbol{b}_1', \ldots, \boldsymbol{b}_n')'$, $\boldsymbol{\varepsilon} = (\boldsymbol{\varepsilon}_1', \ldots, \boldsymbol{\varepsilon}_n')'$, and $\boldsymbol{G} = \mathrm{diag}(\boldsymbol{D}, \ldots, \boldsymbol{D})$ is a $r \times r$ block-diagonal matrix. We assume that the observed data $\boldsymbol{y}$ is generated from (3.1). We also assume $\boldsymbol{D} = \mathrm{diag}(\sigma_1^2, \ldots, \sigma_k^2)$.

Model (3.1) can be re-written as the form

$$\boldsymbol{Y} = \boldsymbol{X}\boldsymbol{\beta} + \sum_{i=1}^{k} \boldsymbol{B}_i \boldsymbol{a}_i + \boldsymbol{\varepsilon}, \tag{3.2}$$

where $\boldsymbol{Z} = (\boldsymbol{B}_1, \ldots, \boldsymbol{B}_k)$ is an $N \times (nk)$ matrix associated with the random effects $\boldsymbol{a} = (\boldsymbol{a}_1', \ldots, \boldsymbol{a}_k')$. Here, $\boldsymbol{a}_i \sim N(0, \sigma_i^2 \boldsymbol{I}_n), i = 1, \ldots, k$ are assumed to be mutually independent and independent of the random error $\boldsymbol{\varepsilon} \sim N(0, \sigma_\varepsilon^2 \boldsymbol{I}_N)$. Then

$$\mathrm{E}(\boldsymbol{Y}) = \boldsymbol{X}\boldsymbol{\beta}, \quad \mathrm{Var}(\boldsymbol{Y}) = \sum_{i=1}^k \sigma_i^2 \boldsymbol{B}_i \boldsymbol{B}_i' + \sigma_\varepsilon^2 \boldsymbol{I}_N \triangleq \sigma_\varepsilon^2 V_y.$$

In the following, we propose a general test for the hypothesis test

$$H_0 : \sigma_i^2 \leqslant \sigma_0^2 \leftrightarrow H_1 : \sigma_i^2 > \sigma_0^2. \tag{3.3}$$

Then we give the fiducial generalized p-value for testing zero variance component when $\sigma_0^2 = 0$.

Let $\boldsymbol{Z}_i^* = (\boldsymbol{B}_1, \ldots, \boldsymbol{B}_{i-1}, \boldsymbol{B}_{i+1}, \ldots, \boldsymbol{B}_k)$ and $\boldsymbol{a}_i^* = (\boldsymbol{a}_1', \ldots, \boldsymbol{a}_{i-1}', \boldsymbol{a}_{i+1}', \ldots, \boldsymbol{a}_k')'$. Then Model (3.2) can be written as the following form:

$$\boldsymbol{Y} = \boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{Z}_i^* \boldsymbol{a}_i^* + \boldsymbol{B}_i \boldsymbol{a}_i + \boldsymbol{\varepsilon}. \tag{3.4}$$

Denote $\Omega(\mathcal{A})$ by the space generated by the matrix/vector $\mathcal{A}$, and assume that $\Omega(\boldsymbol{B}_i) \nsubseteq \Omega(\boldsymbol{X}, \boldsymbol{Z}^*)$. This means that the space generated by $\boldsymbol{B}_i$ is not a subspace of $\Omega(\boldsymbol{X}, \boldsymbol{Z}^*)$, the space generated by $(\boldsymbol{X}, \boldsymbol{Z}^*)$.

3.2 Restricted likelihood ratio test in LME

Recall $V_y = \mathrm{var}(\boldsymbol{Y})/\sigma_\varepsilon^2$. Twice the log-likelihood function of the observations $\boldsymbol{Y}$ for Model (3.2) with parameters $\boldsymbol{\beta}, \sigma_\varepsilon^2, \sigma_i^2$ $(i = 1, \ldots, k)$ is

$$L(\boldsymbol{\beta}, \sigma_\varepsilon^2, \{\sigma_i^2\}_1^k) = -\left[-n \log \sigma_\varepsilon^2 + \log\{\det(V_y)\} + \frac{(\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{\beta})' V_y^{-1} (\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{\beta})}{\sigma_\varepsilon^2} \right].$$

The associated restricted likelihood is

$$\mathrm{RL}(\boldsymbol{\beta}, \sigma_\varepsilon^2, \{\sigma_i^2\}_1^k) = L(\boldsymbol{\beta}, \sigma_\varepsilon^2, \{\sigma_i^2\}_1^k) - \log\{\det(\boldsymbol{X}' V_y^{-1} \boldsymbol{X})\}.$$

The (log) restricted likelihood ratio test corresponding to the hypothesis (3.3) can be expressed as

$$\mathrm{RLRT}_n = \sup_{H_1} \mathrm{RL}(\boldsymbol{\beta}, \sigma_\varepsilon^2, \{\sigma_i^2\}_1^k) - \sup_{H_0} \mathrm{RL}(\boldsymbol{\beta}, \sigma_\varepsilon^2, \{\sigma_i^2\}_1^k).$$

Computing RLRT_n is feasible since one needs only to compute the restricted maximum likelihood with multiple variance components given inequality constrains, though it is not simple. But deriving the null and alternative distributions is very challenging. This challenge becomes more serious when $\sigma_0^2 = 0$ because the parameter under the null hypothesis is on the boundary of the parameter space.

To ease this challenge, Crainiceanu and Ruppert [4] further assumed that $\sigma_i^2 \equiv \sigma_c^2$, and showed that the corresponding exact null distribution of the RLRT_n has the same distribution as the following statistic:

$$\sup_\lambda \left[(N - p) \log \left\{ 1 + \frac{N_N(\lambda)}{D_N(\lambda)} \right\} - \sum_{j=1}^r \log(1 + \lambda \mu_j) \right],$$

where

$$N_N(\lambda) = \sum_{j=1}^r \frac{\lambda \mu_j}{1 + \lambda \mu_j} w_j^2, \quad D_N(\lambda) = \sum_{j=1}^r \frac{w_j^2}{1 + \lambda \mu_j} + \sum_{j=r+1}^{N-p} w_j^2,$$

w_j $(j = 1, \ldots, N - p)$ are i.i.d. $N(0, 1)$, and μ_j $(j = 1, \ldots, r)$ are the eigenvalues of the matrix $\boldsymbol{Z}'\{\boldsymbol{I}_N - \boldsymbol{X}(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}'\}\boldsymbol{Z}$. The distribution of this statistic can be numerically simulated because it depends only on the eigenvalues μ_j, which need to be calculated only once [4].

3.3 Fiducial generalized p-value for LME

We now derive a fiducial generalized p-value for the hypothesis (3.3) using the recipe proposed in Section 2. The procedure can be divided into two steps. In the first step, we derive $\boldsymbol{\Xi}$ required in Theorem 2.2. In the second step, we deduce the fiducial distribution of σ_i^2 and construct a structural equation or a positively weighted structural equation (see below for more details), based on which we obtain the fiducial generalized p-value for the hypothesis (3.3).

Step 1. Denote $r_i = \mathrm{rank}(\boldsymbol{X},\boldsymbol{Z}) - \mathrm{rank}(\boldsymbol{X},\boldsymbol{Z}_i^*)$, and $f = N - \mathrm{rank}(\boldsymbol{X},\boldsymbol{Z})$. It is easy to see that $r_i > 0$ and $f > 0$. Let $P_{(\boldsymbol{X},\boldsymbol{Z})}$ and $P_{(\boldsymbol{X},\boldsymbol{Z}_i^*)}$ denote the orthogonal projection matrixes onto the vector space generated by the columns of $[\boldsymbol{X},\boldsymbol{Z}]$ and $[\boldsymbol{X},\boldsymbol{Z}_i^*]$, respectively. It is easy to see that $P_{(\boldsymbol{X},\boldsymbol{Z})} - P_{(\boldsymbol{X},\boldsymbol{Z}_i^*)}$ is an idempotent matrix, and $\mathrm{rank}\{P_{(\boldsymbol{X},\boldsymbol{Z})} - P_{(\boldsymbol{X},\boldsymbol{Z}_i^*)}\} = r_i$. Let A_i be an $r_i \times N$ matrix such that $A_iA_i{}' = \boldsymbol{I}_{r_i}$ and $A_i'A_i = P_{(\boldsymbol{X},\boldsymbol{Z})} - P_{(\boldsymbol{X},\boldsymbol{Z}_i^*)}$. Multiplying A_i on both sides of (3.4), we have

$$
\begin{aligned}
&A_i\boldsymbol{Y} = A_i\boldsymbol{B}_i\boldsymbol{a}_i + A_i\boldsymbol{\varepsilon} \sim N(0, \sigma_i^2 C_i + \sigma_\varepsilon^2 \boldsymbol{I}_{r_i}),\\
&\boldsymbol{V}_0 = \boldsymbol{Y}'(\boldsymbol{I}_N - P_{(\boldsymbol{X},\boldsymbol{Z})})\boldsymbol{Y} \sim \sigma_\varepsilon^2\chi_f^2,
\end{aligned} \tag{3.5}
$$

where $C_i = A_i\boldsymbol{B}_i\boldsymbol{B}_i'A_i'$, and $A_i\boldsymbol{Y}$ and $\boldsymbol{V}_0$ are mutually independent. Let $\lambda_i^{(1)} > \lambda_i^{(2)} > \cdots > \lambda_i^{(d_i)} > 0$ be the distinct eigenvalues of C_i with multiplicities $r_i^{(1)}, \ldots, r_i^{(d_i)}$, where $\sum_{j=1}^{d_i} r_i^{(j)} = r_i$. Let $H_i = [H_i^{(1)}, \ldots, H_i^{(d_i)}]$ be an $r_i \times r_i$ orthogonal matrix such that

$$
H_iC_iH_i' = \mathrm{diag}\{\lambda_i^{(1)}\boldsymbol{I}_{r_i^{(1)}}, \ldots, \lambda_i^{(d_i)}\boldsymbol{I}_{r_i^{(d_i)}}\},
$$

where $H_i^{(j)}$ corresponding to $\lambda_i^{(j)}$ is of size $r_i \times r_i^{(j)}$. Let $r_0 = f$. By (3.5), we see that

$$
\begin{cases}
\boldsymbol{V}_i^{(j)} = \boldsymbol{Y}'A_i'(H_i^{(j)})'H_i^{(j)}A_i\boldsymbol{Y} \sim (\lambda_i^{(j)}\sigma_i^2 + \sigma_\varepsilon^2)\chi^2_{r_i^{(j)}}, \quad j = 1, \ldots, d_i,\\
\boldsymbol{V}_0 \sim \sigma_\varepsilon^2\chi^2_{r_0},
\end{cases} \tag{3.6}
$$

and $\boldsymbol{V}_0, \boldsymbol{V}_i^{(1)}, \ldots, \boldsymbol{V}_i^{(d_i)}$ are mutually independent.

Step 2. Next, we construct structural equations by applying the statistics obtained in Step 1. By (3.6), we have the following structural equations:

$$
\begin{cases}
\boldsymbol{V}_i^{(j)} = (\lambda_i^{(j)}\sigma_i^2 + \sigma_\varepsilon^2)\boldsymbol{U}_i^{(j)}, \quad j = 1, \ldots, d_i,\\
\boldsymbol{V}_0 = \sigma_\varepsilon^2\boldsymbol{U}_0,
\end{cases} \tag{3.7}
$$

where $\boldsymbol{U}_i^{(j)} \sim \chi^2_{r_i^{(j)}}, j = 1, \ldots, d_i$, $\boldsymbol{U}_0 \sim \chi^2_{r_0}$. The above equation provides a structural representation for the observed random vector $\boldsymbol{v}_i = (\boldsymbol{v}_0, \boldsymbol{v}_i^{(1)}, \ldots, \boldsymbol{v}_i^{(d_i)})$ in terms of the random vector $\boldsymbol{U}_i = (\boldsymbol{U}_0, \boldsymbol{U}_i^{(1)}, \ldots, \boldsymbol{U}_i^{(d_i)})$, whose distribution is completely known.

Based on Theorem 2.2, the structural equations should have a unique solution. However, this may not be always true when $d_i \geqslant 2$. We now separately deal with the cases $d_i = 1$ and $d_i \geqslant 2$.

Case 1. $d_i = 1$. The structural equation

$$
\begin{cases}
\boldsymbol{v}_i^{(1)} = (\lambda_i^{(1)}\sigma_i^2 + \sigma_\varepsilon^2)\boldsymbol{u}_i^{(1)},\\
\boldsymbol{v}_0 = \sigma_\varepsilon^2\boldsymbol{u}_0
\end{cases}
$$

has a unique solution in $\mathbb{R}$:

$$
(\sigma_i^2, \sigma_\varepsilon^2) = \left\{\frac{1}{\lambda_i}\left(\frac{\boldsymbol{v}_i^{(1)}}{\boldsymbol{u}_i^{(1)}} - \frac{\boldsymbol{v}_0}{\boldsymbol{u}_0}\right), \frac{\boldsymbol{v}_0}{\boldsymbol{u}_0}\right\}
$$

for each observed $\boldsymbol{v}_i$ and for every $\boldsymbol{u}_i$. Then the fiducial distribution of σ_i^2 is

$$
F_i(t) = \mathrm{P}\left\{\frac{1}{\lambda_i}\left(\frac{\boldsymbol{v}_i^{(1)}}{\boldsymbol{U}_i^{(1)}} - \frac{\boldsymbol{v}_0}{\boldsymbol{U}_0}\right) \leqslant t\right\}.
$$

Correspondingly, the fiducial generalized p-value for the hypothesis (3.3) equals

$$F_i(\sigma_0^2) = \mathrm{P}\biggl(\frac{\boldsymbol{v}_i^{(1)}}{\boldsymbol{U}_i^{(1)}} - \frac{\boldsymbol{v}_0}{\boldsymbol{U}_0} \leqslant \lambda_i \sigma_0^2\biggr).$$

When $\sigma_0^2 = 0$, the corresponding generalized p-value for the hypothesis (3.3) is

$$F_i(0) = \mathrm{P}\biggl(\frac{\boldsymbol{v}_i^{(1)}}{\boldsymbol{U}_i^{(1)}} - \frac{\boldsymbol{v}_0}{\boldsymbol{U}_0} \leqslant 0\biggr) = 1 - F_{r_i^{(1)},f}\biggl(\frac{\boldsymbol{v}_i^{(1)}/r_i^{(1)}}{\boldsymbol{v}_0/f}\biggr),$$

which is identical to the classical F-test.

Case 2. $d_i \geqslant 2$. Note that the structural equations

$$\begin{cases} \boldsymbol{v}_i^{(j)} = (\lambda_i^{(j)}\sigma_i^2 + \sigma_\varepsilon^2)\boldsymbol{u}_i^{(j)}, \quad j = 1, \dots, d_i, \\ \boldsymbol{v}_0 = \sigma_\varepsilon^2 \boldsymbol{u}_0 \end{cases}$$

may have more than one solution for some observed $\boldsymbol{v}_i$ and $\boldsymbol{u}_i$. We now try to determine a proper solution based on the available solutions, which is a combination of statistics $\boldsymbol{V}_i^{(j)}$ with non-negative weights, say $\sum_{j=1}^{d_i} c_i^{(j)} \boldsymbol{V}_i^{(j)}$. For observation $\boldsymbol{v}_i^{(j)}$ of $\boldsymbol{V}_i^{(j)}$, we consider the following structural equation based on (3.7):

$$\begin{cases} \displaystyle\sum_{j=1}^{d_i} c_i^{(j)} \boldsymbol{V}_i^{(j)} = \sum_{j=1}^{d_i} c_i^{(j)} (\lambda_i^{(j)}\sigma_i^2 + \sigma_\varepsilon^2)\boldsymbol{U}_i^{(j)}, \\ \boldsymbol{V}_0 = \sigma_\varepsilon^2 \boldsymbol{U}_0, \end{cases}$$

where $c_i^{(j)}$ are the non-negative weights. We elucidate selection of these weights in Appendix A. Then for observed $\boldsymbol{v}_i^{(j)}$ and $\boldsymbol{u}_i^{(j)}$,

$$\begin{cases} \displaystyle\sum_{j=1}^{d_i} c_i^{(j)} \boldsymbol{v}_i^{(j)} = \sum_{j=1}^{d_i} c_i^{(j)} (\lambda_i^{(j)}\sigma_i^2 + \sigma_\varepsilon^2)\boldsymbol{u}_i^{(j)}, \\ \boldsymbol{v}_0 = \sigma_\varepsilon^2 \boldsymbol{u}_0 \end{cases}$$

has a unique solution for $(\sigma_i^2, \sigma_\varepsilon^2)$ in $\mathbb{R}$:

$$\begin{cases} \sigma_i^2 = \dfrac{\sum_{j=1}^{d_i} c_i^{(j)} \boldsymbol{v}_i^{(j)} - \frac{\boldsymbol{v}_0}{\boldsymbol{u}_0} \sum_{j=1}^{d_i} c_i^{(j)} \boldsymbol{u}_i^{(j)}}{\sum_{j=1}^{d_i} c_i^{(j)} \lambda_i^{(j)} \boldsymbol{u}_i^{(j)}}, \\ \sigma_\varepsilon^2 = \dfrac{\boldsymbol{v}_0}{\boldsymbol{u}_0}. \end{cases}$$

Accordingly the fiducial distribution of σ_i^2 is

$$F_i(t) = \mathrm{P}\biggl\{\frac{\sum_{j=1}^{d_i} c_i^{(j)} \boldsymbol{v}_i^{(j)} - \frac{\boldsymbol{v}_0}{\boldsymbol{U}_0} \sum_{j=1}^{d_i} c_i^{(j)} \boldsymbol{U}_i^{(j)}}{\sum_{j=1}^{d_i} c_i^{(j)} \lambda_i^{(j)} \boldsymbol{U}_i^{(j)}} \leqslant t\biggr\},$$

and the associated generalized p-value for the hypothesis (3.3) is

$$p_i = F_i(\sigma_0^2) = \mathrm{P}\biggl\{\frac{\sum_{j=1}^{d_i} c_i^{(j)} \boldsymbol{v}_i^{(j)}}{\boldsymbol{v}_0} - \frac{\sum_{j=1}^{d_i} c_i^{(j)} \boldsymbol{U}_i^{(j)}}{\boldsymbol{U}_0} \leqslant \frac{\sigma_0^2 \sum_{j=1}^{d_i} c_i^{(j)} \lambda_i^{(j)} \boldsymbol{U}_i^{(j)}}{\boldsymbol{v}_0}\biggr\}.$$

Especially, when $\sigma_0^2 = 0$, the generalized p-value for the hypothesis (3.3) is

$$p_i = F_i(0) = \mathrm{P}\biggl\{\frac{\sum_{j=1}^{d_i} c_i^{(j)} \boldsymbol{U}_i^{(j)}}{\boldsymbol{U}_0} \geqslant \frac{\sum_{j=1}^{d_i} c_i^{(j)} \boldsymbol{v}_i^{(j)}}{\boldsymbol{v}_0}\biggr\} = \mathrm{E}\biggl\{G_f\biggl(\frac{v_0 \sum_{j=1}^{d_i} c_i^{(j)} \boldsymbol{U}_i^{(j)}}{\sum_{j=1}^{d_i} c_i^{(j)} \boldsymbol{v}_i^{(j)}}\biggr)\biggr\}, \tag{3.8}$$

where G_f is the cdf (cumulative distribution function) of the chi-squared distribution with f degrees of freedom and the expectation is taken with respect to the random variables $(\boldsymbol{U}_i^{(1)}, \dots, \boldsymbol{U}_i^{(d_i)})$.

Remark 3.1. When $\sigma_0^2 = 0$, if we simply take $c_j = 1$, the generalized p-value for the hypothesis (3.3) reduces to

$$p_i = \mathrm{P}\left\{\frac{\sum_{j=1}^{d_i} \boldsymbol{U}_i^{(j)}}{\boldsymbol{U}_0} \geqslant \frac{\sum_{j=1}^{d_i} \boldsymbol{v}_i^{(j)}}{\boldsymbol{v}_0}\right\} = 1 - F_{r_i,f}\left(\frac{\sum_{j=1}^{d_i} \boldsymbol{v}_i^{(j)}/r_i}{\boldsymbol{v}_0/f}\right).$$

This is identical to the p-value of the Wald test. However, the power of the Wald test is generally lower than that of other tests such as RLR test as noticed by [25].

Remark 3.2. Our method provides a simple way to obtain the distribution of $\sigma_\varepsilon^2 = \boldsymbol{v}_0/\boldsymbol{u}_0$ and the fiducial distribution of σ_i^2 by combining the multi-structural equations with proper weights. However, Hannig and Iyer [15] used a different strategy. They selected two equations from the available structural equations under their setting and solved for σ_i^2 and σ_ε^2, and plugged the solutions into the remaining equations for conditioning, then calculated the fiducial distributions of σ_i^2 and σ_ε^2 by averaging the results for all possible choices of two structural equations. Their calculations involve evaluations of multiple integrations and are quite complex in implementation.

It is worthwhile to point out that the generalized p-value can be computed exactly, instead of approximately, but they are generally not equal to the conventional p-value because the null distributions of generalized test variables are not uniform. Several papers studied frequentist properties of generalized p-values by simulations (see [19, 21]). It is very interesting and attractive that the type I error of the proposed fiducial generalized p-value (3.8) exactly equals to the nominal level. We can justify this claim as follows.

Proposition 3.3. *When $\sigma_0^2 = 0$, the type* I *error of the fiducial generalized p-value* (3.8) *exactly equals to the nominal level.*

Proof. Let $\widetilde{\boldsymbol{U}}_i$ and $\boldsymbol{U}_i$ be independent and identically distributed. Then by (3.7), we have $\boldsymbol{V}_i^{(j)} = (\lambda_i^{(j)}\sigma_i^2 + \sigma_\varepsilon^2)\widetilde{\boldsymbol{U}}_i^{(j)}$, $j = 1, \ldots, d_i$, and $\boldsymbol{V}_0 = \sigma_\varepsilon^2 \widetilde{\boldsymbol{U}}_0$. For a given level γ, under the null hypothesis $H_0 : \sigma_i^2 = 0$, we have

$$\begin{aligned}\mathrm{P}(p_i \leqslant \gamma) &= \mathrm{P}\left\{\mathrm{P}\left(\frac{\sum_{j=1}^{d_i} c_i^{(j)}\boldsymbol{U}_i^{(j)}}{\boldsymbol{U}_0} \geqslant \frac{\sum_{j=1}^{d_i} c_i^{(j)}\boldsymbol{V}_i^{(j)}}{\boldsymbol{V}_0} \,\middle|\, \boldsymbol{V}_i\right) \leqslant \gamma\right\} \\ &= \mathrm{P}\left\{\mathrm{P}\left(\frac{\sum_{j=1}^{d_i} c_i^{(j)}\boldsymbol{U}_i^{(j)}}{\boldsymbol{U}_0} \geqslant \frac{\sum_{j=1}^{d_i} c_i^{(j)}\widetilde{\boldsymbol{U}}_i^{(j)}}{\widetilde{\boldsymbol{U}}_0} \,\middle|\, \widetilde{\boldsymbol{U}}_i\right) \leqslant \gamma\right\} \\ &= \gamma.\end{aligned}$$

We finish the proof. □

Remark 3.4. A simple non-negative weight is $c_i^{(j)} = \lambda_1^{(j)}$. More details can be found in Appendix A. We use this weight in our following discussions.

Remark 3.5. If we have only one random term in Model (3.2), i.e., $k = 1$, it is easy to obtain the generalized p-value for testing zero-variance component in (3.3). Let $c_i^{(j)} = \lambda_1^{(j)}$. The resulting p-value is

$$p = \mathrm{E}\left\{G_f\left(\frac{\boldsymbol{v}_0 \sum_{j=1}^{d} \lambda_1^{(j)}\boldsymbol{U}_1^{(j)}}{\sum_{j=1}^{d} \lambda_1^{(j)}\boldsymbol{v}_1^{(j)}}\right)\right\}.$$

It is similar to a combined invariant test of [10], which is based on the geometric mean of Wald test and is locally most powerful.

A direct calculation of the fiducial generalized p-value may sometimes be complex when the calculation involves multiple integrations. A simple but effective alternative is to use the Monte Carlo simulation approach as advocated by [36], which is given as follows.

Monte Carlo algorithm. • Compute $P_{\boldsymbol{X},\boldsymbol{Z}}$, $P_{(\boldsymbol{X},\boldsymbol{Z}^*)}$, A_i and H_i. Then compute $\boldsymbol{v}_i^{(j)} = \boldsymbol{y}'A_i'(H_i^{(j)})' H_i^{(j)}A_i\boldsymbol{y}$, $j = 1, \ldots, d_i$, and $\boldsymbol{v}_0 = \boldsymbol{y}'(I - P_{(\boldsymbol{X},\boldsymbol{Z})})\boldsymbol{y}$.

- Generate a $\boldsymbol{u}_l$ randomly from the distribution of $\boldsymbol{U} = (\boldsymbol{U}_0, \boldsymbol{U}_i^{(1)}, \ldots, \boldsymbol{U}_i^{(d_i)})$. Compute

$$t_l = \frac{\sum_{j=1}^{d_i} \lambda_i^{(j)} \boldsymbol{U}_i^{(j)}}{\boldsymbol{U}_0} - \frac{\sum_{j=1}^{d_i} \lambda_i^{(j)} \boldsymbol{v}_i^{(j)}}{\boldsymbol{v}_0}.$$

Repeat M times.

- The simulated generalized p-value is $\#\{t_l \geqslant 0, l = 1, 2, \ldots, M\}/M$ for testing H_0.

4 Testing linearity in additive models

We now apply the proposed test in Section 3 for checking linearity in additive models. Additive modelling, as a dimensional reduction tool for modelling the relationship between a response and multiple predictors, becomes powerful to tackle the "curse of dimensionality" problem, and has been extensively studied in the literature [24].

Assuming that an additive structure is valid, it is often desirable to further simplify it to partial linear additive models (see [17]), which combine both linear components and nonparametric components in the additive setting. This is especially important when it is believed that the response variable Y depends on some independent variables linearly and others nonlinearly. As a consequence, the linear coefficients can be estimated at the root-n convergence rate, and interpretation of the effect of linear components is easier and more intuitive than that of additive nonparametric components.

Suppose that the relationship between the response variable Y and covariates $\boldsymbol{X} = (X_1, \ldots, X_p)$ can be represented as a sum of unknown one-dimensional functions of the individual variables; i.e., $Y = \alpha + \sum_{j=1}^p f_j(X_j) + \varepsilon$, where ε is the model error. Assume $\int f_j(x_j)dx_j = 0$ to ensure model identifiability. We intend to test whether f_j is linear. In a discussion of a seminal paper, Brumback et al. [2] pointed out that there is a close relationship between the penalized spline nonparametric additive models and LME; i.e., the estimator of the nonparametric functions is equivalent to estimation of parameters in a LME model. Motivated by this linkage, we develop a testing procedure to check the linearity of $f_j(\cdot)$ by applying the proposed procedure for testing of zero-variance components.

Approximate f_j by $f_j(x; \boldsymbol{\beta}_j) = \beta_{1,j}x + \sum_{k=1}^{K_j} \beta_{1+k,j}(x - \zeta_{kj})_+$, where $\boldsymbol{\beta}_j = (\beta_{1,j}, \beta_{2,j}, \ldots, \beta_{1+K_j,j})'$, $\zeta_{1j} < \cdots < \zeta_{K_jj}$, and $a_+ = \max(a, 0)$ (see [24, pp. 216–218] for more details). Then the estimators $\widehat{\boldsymbol{\beta}}_j$ of $\boldsymbol{\beta}_j$ are defined as the minimizers of

$$\sum_{i=1}^n \left\{ Y_i - \sum_{j=1}^p f_j(X_{ji}; \boldsymbol{\beta}_j) \right\}^2 + \sum_{j=1}^p \alpha_{xj} \sum_{k=1}^{K_j} \beta_{1+k,j}^2, \tag{4.1}$$

where α_{xj} are penalty parameters. The estimators $\widehat{\boldsymbol{\beta}}_j$ based on (4.1) are equivalent to the estimators of $\boldsymbol{\beta}_j$ based on the following LME model:

$$\boldsymbol{Y} = \alpha + \boldsymbol{X}_1\boldsymbol{\beta}_1 + \boldsymbol{\Xi}(x_1)\boldsymbol{b}_1 + \cdots + \boldsymbol{X}_p\boldsymbol{\beta}_p + \boldsymbol{\Xi}(x_p)\boldsymbol{b}_p + \boldsymbol{\varepsilon},$$

where

$$\boldsymbol{X}_j = \begin{pmatrix} X_{1j} \\ X_{2j} \\ \vdots \\ X_{nj} \end{pmatrix}, \quad \boldsymbol{\Xi}(x_j) = \left\{ \begin{matrix} (X_{1j} - \zeta_{1j})_+ & \cdots & (X_{1j} - \zeta_{K_jj})_+ \\ (X_{2j} - \zeta_{1j})_+ & \cdots & (X_{2j} - \zeta_{K_jj})_+ \\ \vdots & \ddots & \vdots \\ (X_{nj} - \zeta_{1j})_+ & \cdots & (X_{nj} - \zeta_{K_jj})_+ \end{matrix} \right\},$$

$\boldsymbol{Y} = (Y_1, Y_2, \ldots, Y_n)'$, and $\boldsymbol{b}_j = (b_{1j}, \ldots, b_{K_jj})' \sim N(0, \sigma_{bj}^2)$.

This equivalence implies that the minimizers of (4.1) are identical to the estimators of the standard LME given [2, 5]. Therefore, testing linearity of $f_j(x_j)$ is equivalent to testing $\sigma_{bj}^2 = 0$, which we can achieve by applying the proposed procedure in Section 3.

5 Simulation studies

To evaluate the performance of the proposed fiducial generalized p-value (refer as FG test hereafter), Monte Carlo simulations were used to compare the empirical power of FG test to that of the existing RLR test. Our simulation studies are designed as follows. The first example is used to investigate the test for zero-variance slope in a LME model, and the second example is dedicated to test nonlinearity of nonparametric functions in an additive nonparametric model.

Example 5.1. In this example, observations are generated from the following model:

$$\boldsymbol{Y}_{ij} = b_{0i} + (1 + b_{1i})x_{ij} + \boldsymbol{\varepsilon}_{ijk}, \quad i = 1, \ldots, g, \quad j = 1, \ldots, n_i,$$

where $b_{0i} \sim N(0,1)$, $b_{1i} \sim N(0,\sigma_1^2)$ and $\boldsymbol{\varepsilon}_{ijk} \sim N(0,1)$, and b_{0i}'s, b_{1i}'s and $\boldsymbol{\varepsilon}_{ijk}$'s are mutually independent. We use $x_{ij} \sim U[0,1]$, and examine four configurations with $g = 5$ or $g = 10$ and $N = \sum_i^g n_i = 30$ and $N = \sum_i^g n_i = 50$. We evaluate the numerical performance of FG and RLR tests for the hypothesis

$$H_0 : \sigma_1^2 = 0 \leftrightarrow H_1 : \sigma_1^2 > 0.$$

In this simulation example, let $\lambda = \sigma_1^2/\sigma_e^2 = \sigma_1^2$, so we could compute the power of test when σ_1^2 changes. We generated 4,000 simulation data sets. For each simulated data set, the Monte Carlo sample size of $M = 5{,}000$ was used to obtain the fiducial generalized p-value of FG test and the p-value of RLR test. The empirical power is the proportion of rejecting the null hypothesis among 4,000 simulation runs. We used the nominal significance level of 0.05 in our simulation studies. For the RLR test, we used lmer( ) from the R-package lme4 to fit the models and the R-package RLRsim was used to obtain the power.

Figure 1 presents the proportions of rejecting the null hypothesis of the two tests for four different settings. Note that when $\sigma_1^2 = 0$, the proportions of rejecting H_0 of two tests for all settings are all close to the nominal level. As σ_1^2 deviates zero, the rejection trend (or the power curves) based on two tests increases with the increase of σ_1^2. But the proposed test wins for all different configurations with significant superiority given small individual observations. For the case where the number of individual observations is large, two methods show similar performance (not presented for space concern).

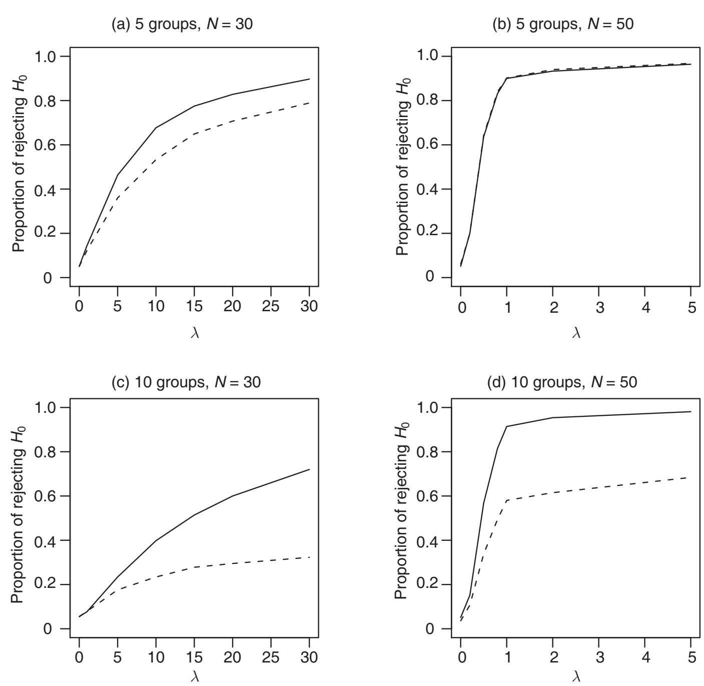

Figure 1 Simulation results for Example 5.1. The empirical power of rejecting null hypothesis for different σ_1^2 under four configurations (solid line for FG test; dashed lines for RLR test)

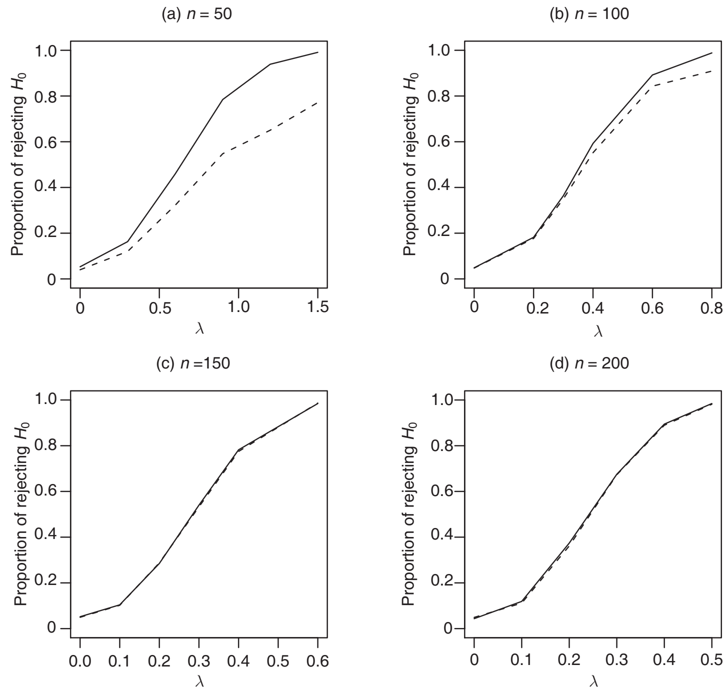

Figure 2 Simulation results for Example 5.2. The empirical power of rejecting null hypothesis for different λ values for each sample size (solid line for FG test; dashed lines for RLR test)

Example 5.2. In this example, we evaluate the performance of the proposed approach in Appendix B. Observations are generated from a two-regressor model $\boldsymbol{Y} = f_1(x) + f_2(z) + \varepsilon$ with $f_1(x) = 2x + \lambda\sin(\pi x)$ and $f_2(z) = \cos(5\pi z)$, where $\varepsilon \sim N(0, 0.5^2)$. We are interested in the power of FG and RLR tests to detect the nonlinearity of $f_1(x)$ when $\lambda \neq 0$. Both x and z are equally spaced on $[0, 1]$. We consider four sample sizes: $n = 50$, $n = 100$, $n = 150$ and $n = 200$.

In this experiment, $K_x = 15$ and $K_z = 17$ were used to fit the model. At each configuration and observation sample size, we generated 2,000 simulation data sets. For each simulated data set, the Monte Carlo sample size of $M = 5{,}000$ was used to obtain the fiducial generalized p-value of FG test and the p-value of RLR test. The simulation results are summarized in Figure 2. When $\lambda = 0$, the proportions of rejecting the linearity of $f_1(x)$ of two tests for all settings are all close to the nominal level again. Not surprisingly, the power of the two tests increases as λ becomes larger. With moderate or large sample sizes, the performance of the two tests is similar. However, the superiority of FG test to RLR test is remarkable when the sample size is small. This fact can be easily seen from (a) and (b) of Figure 2, which indicates that our FG test is more powerful.

6 A nutritional study

Observational studies have shown that there is a direct relationship between beta-carotene and cancers such as lung, colon, breast, and prostate cancer (see [11]). Beta-carotene can effectively prevent cancers since beta-carotene has powerful antioxidant properties and can help clean the body of free radicals that can cause cancer. Sufficient beta-carotene supply can also strengthen the body's autoimmune system, making it more effective in fighting degenerative diseases such as cancer. It is therefore interesting to study the relationship between serum concentrations of beta-carotene and other factors such as age, smoking status, alcohol consumption, and dietary intake because this information may be potentially useful in clinical decision-making and individualization of therapy.

We now illustrate the proposed procedure by analyzing real data from a nutritional epidemiology study (see [22] for a detailed description of the study). A preliminary examination suggested that plasma

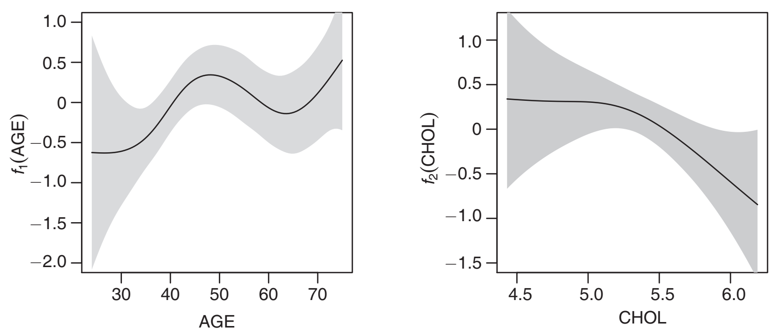

Figure 3 The patterns of AGE and CHOL with ± s.e. for the nutritional dataset

beta-carotene levels linearly depend on CALORIES (number of calories consumed per day), FAT (grams of fat consumed per day), SMOKE (smoked/smoke, never smoked), ALCOHOL (number of alcoholic drinks consumed per week), but possibly nonlinearly depend on CHOL (cholesterol consumed mg per day) and AGE. In this section, we used FG and RLR tests to examine the linearity of CHOL and AGE by analyzing a dataset with 50 observations, i.e., we test linearity of the functions $f_1(\text{AGE})$ and $f_2(\text{CHOL})$ in the following model:

$$\begin{aligned}\log(\text{beta-carotene}) = \beta_0 + \beta_1\text{CALORIES} + \beta_2\text{FAT} + \beta_3\text{ALCOHOL} + \beta_4\text{SMOKE}\\ + f_1(\text{AGE}) + f_2(\text{CHOL}) + \varepsilon. \end{aligned} \tag{6.1}$$

We apply the FG and RLR tests to the model with $K_{\text{AGE}} = K_{\text{CHOL}} = 12$. When testing the linearity of $f_1(\text{AGE})$, we obtained p-values of 0.0015 and 0.198 for the FG and RLR tests, respectively. When testing the linearity of $f_2(\text{CHOL})$, we obtained p-values of 0.0175 and 0.2016 for the FG and RLR tests, respectively. The two tests produce inconsistent conclusions, i.e., the RLR test indicates both AGE and CHOL are linearly related beta-carotene levels, while the proposed FG test obtained an opposite conclusion. Based on our simulation results, we favor the conclusion drawn from the proposed test. To verify this statement, we show the estimated curves of the two nonparametric components, AGE and CHOL, in Figure 3. The patterns seem to support that both AGE and CHOL should be nonlinear.

7 Discussion

Hypothesis testing for zero-variance random components in linear mixed-effects models is a long-standing problem. We combined the concepts of generalized p-values and fiducial inference and derived a general recipe to construct a new testing procedure. The proposed test possesses a number of desirable properties and is easy to implement. Furthermore, the proposed method can be used to test the linearity of nonparametric functions in additive nonparametric models. We also compared our method with a recently proposed likelihood based method, the RLR test. We found out that the performance of the proposed test is as good as the RLR test in large sample sizes, and is better than the RLR test in small sample sizes in terms of the empirical power. Most importantly, we also showed that the actual size of the proposed generalized p-value test exactly equals the nominal level.

It is worthy pointing out that the generalized p-value may not be unique because there may exist different kinds of structure equations, which may result in different generalized p-values. How to find the optimal generalized p-value is warranted as a future study, but beyond the scope of this paper.

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Appendix A Selection of non-negative weights

To obtain proper weights c_j for $j = 1, \dots, d_i$ when $d_i \geqslant 2$, we propose the following procedure. Presume that σ_ε^2 is known. We can derive an unbiased estimator for σ_i^2 from the j-th equation (3.7), $\hat{\sigma}_i^{2(j)} = 1/\lambda_i^{(j)} \cdot (\boldsymbol{V}_i^{(j)}/r_i^{(j)} - \sigma_\varepsilon^2)$. Note that the variance of $\hat{\sigma}_i^{2(j)}$, $D(\hat{\sigma}_i^{2(j)})$, equals $2(\lambda_i^{(j)}\sigma_i^2 + \sigma_\varepsilon^2)^2/(r_i^{(j)}(\lambda_i^{(j)})^2)$, which approaches to $2\sigma_\varepsilon^2/(r_i^{(j)}(\lambda_i^{(j)})^2)$ when $\sigma_i^2 \to 0$. We therefore suggest to estimate σ_i^2 by

$$\hat{\sigma}_i^2 = \sum_{j=1}^{d_i} \frac{\hat{\sigma}_i^{2(j)}}{D(\hat{\sigma}_i^{2(j)})} \Bigg/ \sum_{j=1}^{d_i} \frac{1}{D(\hat{\sigma}_i^{2(j)})},$$

which approaches to

$$\frac{1}{\sum_{j=1}^{d_i}(\lambda_i^{(j)})^2 r_i^{(j)}} \sum_{j=1}^{d_i} (\lambda_i^{(j)}\boldsymbol{V}_i^{(j)} - \lambda_i^{(j)} r_i^{(j)} \sigma_\varepsilon^2) \quad \text{when} \quad \sigma_i^2 \to 0.$$

Note that σ_ε^2 can be estimated by $\hat{\sigma}_\varepsilon^2 = \boldsymbol{V}_0/r_0$, which can substitute into the above formula to get an estimator of σ_i^2 when σ_i^2 is small,

$$\hat{\sigma}_i^{2*} = \frac{1}{\sum_{j=1}^{d_i}(\lambda_i^{(j)})^2 r_i^{(j)}} \sum_{j=1}^{d_i} \left(\lambda_i^{(j)}\boldsymbol{V}_i^{(j)} - \frac{\lambda_i^{(j)} r_i^{(j)}}{r_0}\boldsymbol{V}_0\right).$$

From (3.8), we take $c_i^{(j)} = \lambda_i^{(j)}$ for $j = 1, 2, \dots, d_i$ as our weights. The resulting generalized p-value for the hypothesis (3.3) is

$$p_i = \mathrm{P}\left\{ \frac{\sum_{j=1}^{d_i} \lambda_i^{(j)} \boldsymbol{v}_i^{(j)}}{\boldsymbol{v}_0} - \frac{\sum_{j=1}^{d_i} \lambda_i^{(j)} \boldsymbol{U}_i^{(j)}}{\boldsymbol{U}_0} \leqslant \frac{\sigma_0^2 \sum_{j=1}^{d_i} \lambda_i^{(j)} \lambda_i^{(j)} \boldsymbol{U}_i^{(j)}}{\boldsymbol{v}_0} \right\}.$$

When $\sigma_0^2 = 0$, the proposed generalized p-value is

$$p_i = \mathrm{E}\left[G_f \left\{ \frac{\boldsymbol{v}_0 \sum_{j=1}^{d_i} \lambda_i^{(j)} \boldsymbol{U}_i^{(j)}}{\sum_{j=1}^{d} \lambda_i^{(j)} \boldsymbol{v}_i^{(j)}} \right\} \right].$$

Appendix B The application of fiducial generalized *p*-value in the two-way ANOVA model

In this appendix, we illustrate how to use Theorem 2.2 to obtain a fiducial generalized p-value for the two-way ANOVA model.

Consider the ANOVA model

$$\boldsymbol{Y}_{ijk} = \mu + \alpha_i + \beta_j + (\alpha\beta)_{ij} + \boldsymbol{\varepsilon}_{ijk}, \quad k = 1, \dots, c, \quad i = 1, \dots, a, \quad j = 1, \dots, b,$$

where α_i is the fixed effect, β_j and $(\alpha\beta)_{ij}$ are the random effects, following $N(0, \sigma_\beta^2)$ and $N(0, \sigma_{\alpha\beta}^2)$, respectively, and $\boldsymbol{\varepsilon}_{ijk} \sim N(0, \sigma_\varepsilon^2)$. β_j's, $(\alpha\beta)_{ij}$'s and $\boldsymbol{\varepsilon}_{ijk}$'s are mutually independent. We are interested in hypothesis testing

$$H_0 : f(\sigma_\beta^2, \sigma_{\alpha\beta}^2) \leqslant \delta \;\leftrightarrow\; H_0 : f(\sigma_\beta^2, \sigma_{\alpha\beta}^2) > \delta,$$

where $f(\sigma_\beta^2, \sigma_{\alpha\beta}^2)$ is a function of σ_β^2 and $\sigma_{\alpha\beta}^2$, and $f(\sigma_\beta^2, \sigma_{\alpha\beta}^2) \in [\theta_1, \theta_2]$.

Write

$$SS_1 = ac\sum_{j=1}^{b}(\overline{Y}_j - \overline{\boldsymbol{Y}})^2, \quad SS_2 = c\sum_{i=1}^{a}\sum_{j=1}^{b}(\overline{\boldsymbol{Y}}_{ij} - \overline{\boldsymbol{Y}}_i - \overline{\boldsymbol{Y}}_j + \overline{\boldsymbol{Y}})^2$$

and

$$SS_3 = \sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{c}(\boldsymbol{Y}_{ijk} - \overline{\boldsymbol{Y}}_{ij})^2,$$

where $\overline{\boldsymbol{Y}}_i = \sum_{j=1}^{b}\sum_{k=1}^{c}(\boldsymbol{Y}_{ijk})/(bc)$, $\overline{\boldsymbol{Y}}_j = \sum_{i=1}^{a}\sum_{k=1}^{c}(\boldsymbol{Y}_{ijk})/(ac)$, $\overline{\boldsymbol{Y}}_{ij} = \sum_{k=1}^{c}(\boldsymbol{Y}_{ijk})/c$, and $\overline{\boldsymbol{Y}} = \sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{c}(\boldsymbol{Y}_{ijk})/(abc)$. Note that $SS_i \sim \theta_i\chi^2_{n_i}$, and SS_i's are mutually independent for $i = 1, 2, 3$, where $\theta_1 = ac\sigma^2_\beta + c\sigma^2_{\alpha\beta} + \sigma^2_\varepsilon$, $\theta_2 = c\sigma^2_{\alpha\beta} + \sigma^2_\varepsilon$, $\theta_3 = \sigma^2_\varepsilon$, $n_1 = b-1$, $n_2 = (a-1)(b-1)$, $n_3 = ab(c-1)$. Let $\boldsymbol{U}_i \sim \chi^2_{n_i}$. Then we have the following structural equations:

$$SS_i = \theta_i\boldsymbol{U}_i, \quad \text{for} \quad i = 1, 2, 3.$$

Let ss_i be the observed value of SS_i. Then for each $\boldsymbol{u} = (\boldsymbol{u}_1, \boldsymbol{u}_2, \boldsymbol{u}_3)$, the equations $ss_i = \theta_i\boldsymbol{u}_i$, $i = 1, 2, 3$, have the solutions of $(\theta_1, \theta_2, \theta_3)$, i.e.,

$$\theta_i = \frac{ss_i}{\boldsymbol{u}_i}, \quad \text{for} \quad i = 1, 2, 3.$$

Note that $\sigma^2_\beta = (\theta_1 - \theta_2)/(ac), \sigma^2_{\alpha\beta} = (\theta_2 - \theta_3)/c$. Let $\delta_1 = \min(\sigma^2_\alpha, \sigma^2_{\alpha\beta})$ and $\delta_2 = \max(\sigma^2_\alpha, \sigma^2_{\alpha\beta})$. Define

$$\begin{aligned} & f^*\left(\frac{1}{ac}\left(\frac{ss_1}{\boldsymbol{U}_1} - \frac{ss_2}{\boldsymbol{U}_2}\right), \frac{1}{c}\left(\frac{ss_2}{\boldsymbol{U}_2} - \frac{ss_3}{\boldsymbol{U}_3}\right)\right) \\ &\quad = \min\left[\max\left\{\delta_1, f\left(\frac{1}{ac}\left(\frac{ss_1}{\boldsymbol{U}_1} - \frac{ss_2}{\boldsymbol{U}_2}\right), \frac{1}{c}\left(\frac{ss_2}{\boldsymbol{U}_2} - \frac{ss_3}{\boldsymbol{U}_3}\right)\right), \delta_2\right\}\right]. \end{aligned}$$

It follows from Theorem 2.2 that the generalized test variable is given as

$$\begin{aligned} \boldsymbol{R} &= \delta - f^*\left(\frac{1}{ac}\left(\theta_1\frac{ss_1}{SS_1} - \theta_2\frac{ss_2}{SS_2}\right), \frac{1}{c}\left(\theta_2\frac{ss_2}{SS_2} - \theta_3\frac{ss_3}{SS_3}\right)\right) \\ &= \delta - f^*\left(\frac{1}{ac}\left(\frac{ss_1}{\boldsymbol{U}_1} - \frac{ss_2}{\boldsymbol{U}_2}\right), \frac{1}{c}\left(\frac{ss_2}{\boldsymbol{U}_2} - \frac{ss_3}{\boldsymbol{U}_3}\right)\right). \end{aligned}$$

As a consequence, the generalized p-value is

$$p = \mathrm{P}\left\{f\left(\frac{1}{ac}\left(\frac{ss_1}{\boldsymbol{U}_1} - \frac{ss_2}{\boldsymbol{U}_2}\right), \frac{1}{c}\left(\frac{ss_2}{\boldsymbol{U}_2} - \frac{ss_3}{\boldsymbol{U}_3}\right)\right) \leqslant \delta\right\}.$$

If $f(\sigma^2_\beta, \sigma^2_{\alpha\beta}) = \sigma^2_\beta + \sigma^2_{\alpha\beta}$, this generalized p-value can be simplified as

$$p = \mathrm{P}\left\{\frac{1}{ac}\left(\frac{ss_1}{\boldsymbol{U}_1} + (a-1)\frac{ss_2}{\boldsymbol{U}_2} - a\frac{ss_3}{\boldsymbol{U}_3}\right) \leqslant \delta\right\},$$

and if $f(\sigma^2_\beta, \sigma^2_{\alpha\beta}) = \sigma^2_{\alpha\beta}$, this generalized p-value can be further simplified as

$$p = \mathrm{P}\left\{\frac{1}{c}\left(\frac{ss_2}{\boldsymbol{U}_2} - \frac{ss_3}{\boldsymbol{U}_3}\right) \leqslant \delta\right\},$$

which is the same as what [35] obtained. Hence, we have demonstrated that Theorem 2.2 can be easily used to derive a general test to obtain a generalized p-value for hypothesis tests.

We now apply the idea developed in Section 3 to derive the fiducial generalized p-value. Write $N = abc$. Let $\boldsymbol{Y} = (\boldsymbol{Y}_{111}, \ldots, \boldsymbol{Y}_{11c}, \ldots, \boldsymbol{Y}_{ab1}, \ldots, \boldsymbol{Y}_{abc})'$, $\alpha = (\mu, \alpha_1, \ldots, \alpha_a)'$, $\beta = (\beta_1, \ldots, \beta_b)'$, $\alpha\beta = ((\alpha\beta)_{11}, \ldots, (\alpha\beta)_{1b}, \ldots, (\alpha\beta)_{a1}, \ldots, (\alpha\beta)_{ab})'$, the model can be rewritten as

$$\boldsymbol{Y} = \boldsymbol{X}\alpha + \boldsymbol{B}_1\beta + \boldsymbol{B}_2(\alpha\beta) + \boldsymbol{\varepsilon}.$$

Here, $\boldsymbol{X} = (1_N, (\boldsymbol{I}_a \otimes 1_b \otimes 1_c))$, $\boldsymbol{B}_1 = 1_a \otimes \boldsymbol{I}_b \otimes 1_c$, $\boldsymbol{B}_2 = \boldsymbol{I}_a \otimes \boldsymbol{I}_b \otimes 1_c$. So we see that $\Omega(\boldsymbol{B}_2) \nsubseteq \Omega(\boldsymbol{X}, \boldsymbol{B}_1)$. Note that $P_{(\boldsymbol{X},\boldsymbol{B}_1)} = \boldsymbol{I}_a \otimes \boldsymbol{I}_b \times \frac{1}{c}\boldsymbol{J}_c - (\boldsymbol{I}_a - \frac{1}{a}\boldsymbol{J}_a) \otimes (\boldsymbol{I}_b - \frac{1}{b}\boldsymbol{J}_b) \otimes \frac{1}{c}\boldsymbol{J}_c$, and $P_{(\boldsymbol{X},\boldsymbol{B}_1,\boldsymbol{B}_2)} = \boldsymbol{I}_a \otimes \boldsymbol{I}_b \otimes \frac{1}{c}\boldsymbol{J}_c$. Some direct calculations yield $\mathrm{rank}\{P_{(\boldsymbol{X},\boldsymbol{B}_1,\boldsymbol{B}_2)} - P_{(\boldsymbol{X},\boldsymbol{B}_1)}\} = (a-1)(b-1) = r$ and $\mathrm{rank}\{\boldsymbol{I}_N - P_{(\boldsymbol{X},\boldsymbol{B}_1,\boldsymbol{B}_2)}\}$

$= ab(c-1) = f$. Furthermore, $\boldsymbol{B}_2\{P_{(\boldsymbol{X},\boldsymbol{B}_1,\boldsymbol{B}_2)} - P_{(\boldsymbol{X},\boldsymbol{B}_1)}\} = c\{P_{(\boldsymbol{X},\boldsymbol{B}_1,\boldsymbol{B}_2)} - P_{(\boldsymbol{X},\boldsymbol{B}_1)}\}$. Then, if A satisfies $AA' = \boldsymbol{I}_r$ and $A'A = P_{(\boldsymbol{X},\boldsymbol{B}_1,\boldsymbol{B}_2)} - P_{(\boldsymbol{X},\boldsymbol{B}_1)}$, there exists an orthogonal matrix H such that $HA\boldsymbol{B}_2\boldsymbol{B}_2'A'H' = c\boldsymbol{I}_r$.

Using the expression given in (3.8), a direct simplification yields the fiducial generalized p-value for testing $H_0 : \sigma^2_{\alpha\beta} = 0 \leftrightarrow H_1 : \sigma^2_{\alpha\beta} > 0$ as

$$p = \mathrm{P}\left\{\frac{1}{c}\left(\frac{\boldsymbol{v}_1}{\chi^2_r} - \frac{\boldsymbol{v}_0}{\chi^2_f}\right) \leqslant 0\right\},$$

where $\boldsymbol{v}_1 = \boldsymbol{y}'A'A\boldsymbol{y} = ss_2$ and $\boldsymbol{v}_0 = \boldsymbol{y}'(\boldsymbol{I} - P_{(\boldsymbol{X},\boldsymbol{B}_1,\boldsymbol{B}_2)})\boldsymbol{y} = ss_3$. This is identical to what [35] gave.