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Supplementary material for Multiple linear regression with compositional response and covariates

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In this supplemental material, the proofs of Theorem 3.1, Theorem 3.2, Theorem 3.3 and Theorem 3.4 are presented in Appendix A, Appendix B, Appendix C and Appendix D, respectively.

Appendix A. Proof of Theorem 3.1

It follows from Equation (8) that

$$\begin{cases} \text{ilr}(\mathbf{u}_{ki})(\text{ilr}(\mathbf{v}_i))^T = \mathbf{W}_{D_k}^T \log(\mathbf{u}_{ki})(\log(\mathbf{v}_i))^T \mathbf{W}_L, \\ \text{ilr}(\mathbf{u}_{ji})(\text{ilr}(\mathbf{u}_{ki}))^T = \mathbf{W}_{D_j}^T \log(\mathbf{u}_{ji})(\log(\mathbf{u}_{ki}))^T \mathbf{W}_{D_k}. \end{cases}$$

Thus Equation (14) can be deduced to

$$\begin{pmatrix} n & \sum_{i=1}^n (\log(\mathbf{u}_{1i}))^T & \cdots & \sum_{i=1}^n (\log(\mathbf{u}_{qi}))^T \\ \sum_{i=1}^n \log(\mathbf{u}_{1i}) & \sum_{i=1}^n \log(\mathbf{u}_{1i})(\log(\mathbf{u}_{1i}))^T & \cdots & \sum_{i=1}^n \log(\mathbf{u}_{1i})(\log(\mathbf{u}_{qi}))^T \\ \sum_{i=1}^n \log(\mathbf{u}_{2i}) & \sum_{i=1}^n \log(\mathbf{u}_{2i})(\log(\mathbf{u}_{1i}))^T & \cdots & \sum_{i=1}^n \log(\mathbf{u}_{2i})(\log(\mathbf{u}_{qi}))^T \\ \vdots & \vdots & \ddots & \vdots \\ \sum_{i=1}^n \log(\mathbf{u}_{qi}) & \sum_{i=1}^n \log(\mathbf{u}_{qi})(\log(\mathbf{u}_{1i}))^T & \cdots & \sum_{i=1}^n \log(\mathbf{u}_{qi})(\log(\mathbf{u}_{qi}))^T \end{pmatrix} \\ \times \begin{pmatrix} \mathbf{b}_0^T \\ \mathbf{W}_{D_1} \mathbf{B}_1^T \\ \vdots \\ \mathbf{W}_{D_q} \mathbf{B}_q^T \end{pmatrix} = \begin{pmatrix} \sum_{i=1}^n (\log(\mathbf{v}_i))^T \mathbf{W}_L \\ \sum_{i=1}^n \log(\mathbf{u}_{1i})(\log(\mathbf{v}_i))^T \mathbf{W}_L \\ \sum_{i=1}^n \log(\mathbf{u}_{2i})(\log(\mathbf{v}_i))^T \mathbf{W}_L \\ \vdots \\ \sum_{i=1}^n \log(\mathbf{u}_{qi})(\log(\mathbf{v}_i))^T \mathbf{W}_L \end{pmatrix}. \quad (\text{A1})$$

If both sides of Equation (A1) are multiplied from the right-hand side by matrix $\mathbf{W}_L^T$, since $\mathbf{W}_L \mathbf{W}_L^T = \mathbf{G}_L$, we can get the same solution as Equation (12), so

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$$\begin{cases} (\log(\mathbf{a}_0))^T \mathbf{G}_L = \mathbf{b}_0^T \mathbf{W}_L^T, \\ \mathbf{A}_j^T = \mathbf{W}_{D_j} \mathbf{B}_j^T \mathbf{W}_L^T \quad (j = 1, 2, \dots, q). \end{cases} \implies \begin{cases} \mathbf{b}_0 = \text{ilr}(\mathbf{a}_0), \\ \mathbf{B}_j = \mathbf{W}_L^T \mathbf{A}_j \mathbf{W}_{D_j} \quad (j = 1, 2, \dots, q). \end{cases} \quad (\text{A2})$$

In fact, if we take ilr coordinates on both sides of Equation (10), according to Property 2.3 (2), we have

$$\begin{aligned} \text{ilr}(\mathbf{v}_i) &= \text{ilr}(\mathbf{a}_0 \oplus \mathbf{A}_1 \boxminus \mathbf{u}_{1i} \oplus \dots \oplus \mathbf{A}_q \boxminus \mathbf{u}_{qi} \oplus \varepsilon_i) \\ &= \text{ilr}(\mathbf{a}_0) + \text{ilr}(\mathbf{A}_1 \boxminus \mathbf{u}_{1i}) + \dots + \text{ilr}(\mathbf{A}_q \boxminus \mathbf{u}_{qi}) + \text{ilr}(\varepsilon_i) \\ &= \text{ilr}(\mathbf{a}_0) + \mathbf{W}_L^T \mathbf{A}_1 \mathbf{W}_{D_1} \text{ilr}(\mathbf{u}_{1i}) + \dots + \mathbf{W}_L^T \mathbf{A}_q \mathbf{W}_{D_q} \text{ilr}(\mathbf{u}_{qi}) + \text{ilr}(\varepsilon_i). \end{aligned}$$

Corresponding to model in Equation (13), we can get the same results with Equation (A2), therefore, $\mathbf{a}_0 = \text{ilr}^{-1}(\mathbf{b}_0)$, $\mathbf{A}_j = \mathbf{W}_L \mathbf{B}_j \mathbf{W}_{D_j}^T$ ($j = 1, 2, \dots, q$).

Appendix B. Proof of Theorem 3.2

For any composition $\mathbf{v} \in \mathcal{S}^L$, by Equation (8), we have that

$$\text{ilr}(\mathbf{v}) = \mathbf{W}_L^T \text{clr}(\mathbf{v}) = \mathbf{W}_L^T \text{clr}(\mathbf{P}_{L,l_0}^T \mathbf{v}^{(l_0)}) = \mathbf{W}_L^T \mathbf{P}_{L,l_0}^T \text{clr}(\mathbf{v}^{(l_0)}) = \mathbf{W}_L^T \mathbf{P}_{L,l_0}^T \mathbf{W}_L \text{ilr}(\mathbf{v}^{(l_0)}),$$

then the model in Equation (13) can be deduced to

$$\begin{aligned} \mathbf{W}_L^T \mathbf{P}_{L,l_0}^T \mathbf{W}_L \text{ilr}(\mathbf{v}_i^{(l_0)}) &= \mathbf{b}_0 + \mathbf{B}_1 \mathbf{W}_{D_1}^T \mathbf{P}_{D_1,l_1}^T \mathbf{W}_{D_1} \text{ilr}(\mathbf{u}_{1i}^{(l_1)}) \\ &\quad + \dots + \mathbf{B}_q \mathbf{W}_{D_q}^T \mathbf{P}_{D_q,l_q}^T \mathbf{W}_{D_q} \text{ilr}(\mathbf{u}_{qi}^{(l_q)}) + \text{ilr}(\varepsilon_i). \end{aligned} \quad (\text{B1})$$

If both sides of Equation (B1) are multiplied from the left-hand side by matrix $\mathbf{W}_L^T \mathbf{P}_{L,l_0} \mathbf{W}_L$, by Property 2.1, we obtain that

$$\begin{aligned} \text{ilr}(\mathbf{v}_i^{(l_0)}) &= \mathbf{W}_L^T \mathbf{P}_{L,l_0} \mathbf{W}_L \mathbf{b}_0 + \mathbf{W}_L^T \mathbf{P}_{L,l_0} \mathbf{W}_L \mathbf{B}_1 \mathbf{W}_{D_1}^T \mathbf{P}_{D_1,l_1}^T \mathbf{W}_{D_1} \text{ilr}(\mathbf{u}_{1i}^{(l_1)}) + \dots \\ &\quad + \mathbf{W}_L^T \mathbf{P}_{L,l_0} \mathbf{W}_L \mathbf{B}_q \mathbf{W}_{D_q}^T \mathbf{P}_{D_q,l_q}^T \mathbf{W}_{D_q} \text{ilr}(\mathbf{u}_{qi}^{(l_q)}) + \mathbf{W}_L^T \mathbf{P}_{L,l_0} \mathbf{W}_L \text{ilr}(\varepsilon_i). \end{aligned}$$

Compared with model in Equation (15), it is clear that $\mathbf{b}_0^{(l_0)} = \mathbf{W}_L^T \mathbf{P}_{L,l_0} \mathbf{W}_L \mathbf{b}_0$, $\mathbf{B}_j^{(l_0,l_j)} = \mathbf{W}_L^T \mathbf{P}_{L,l_0} \mathbf{W}_L \mathbf{B}_j \mathbf{W}_{D_j}^T \mathbf{P}_{D_j,l_j}^T \mathbf{W}_{D_j}$ ($j = 1, 2, \dots, q$).

Appendix C. Proof of Theorem 3.3

Without loss of generality, suppose that $l_0 = l_1 = \dots = l_q = 1$, the model in Equation (17) is simplified to $E(\mathbf{Y}|\mathbf{Z}) = \mathbf{Z}\boldsymbol{\beta}$. When composition $\mathbf{u}_j$ ($j = 1, 2, \dots, q$) is permuted through a $D_j \times D_j$ permutation matrix $\mathbf{P}_j$, we get the regression equation

$$E(\mathbf{Y}|\mathbf{Z}^{(\mathbf{P})}) = \mathbf{Z}^{(\mathbf{P})} \boldsymbol{\beta}^{(\mathbf{P})}, \quad (\text{C1})$$

where $\mathbf{Z}^{(\mathbf{P})} = (\mathbf{z}_1^{(\mathbf{P})}, \mathbf{z}_2^{(\mathbf{P})}, \dots, \mathbf{z}_n^{(\mathbf{P})})^T$, $\mathbf{z}_i^{(\mathbf{P})} = (1, (\text{ilr}(\mathbf{P}_1 \mathbf{u}_{1i}))^T, (\text{ilr}(\mathbf{P}_2 \mathbf{u}_{2i}))^T, \dots, (\text{ilr}(\mathbf{P}_q \mathbf{u}_{qi}))^T)^T$, $\beta^{(\mathbf{P})}$ is the regression coefficient vector. By Equation (8), we have

$$\text{ilr}(\mathbf{P}_j \mathbf{u}_{ji}) = \mathbf{W}_{D_j}^T \text{clr}(\mathbf{P}_j \mathbf{u}_{ji}) = \mathbf{W}_{D_j}^T \mathbf{P}_j \text{clr}(\mathbf{u}_{ji}) = \mathbf{W}_{D_j}^T \mathbf{P}_j \mathbf{W}_{D_j} \text{ilr}(\mathbf{u}_{ji}),$$

Denote a $(D+1) \times (D+1)$ matrix

$$\mathbf{P} = \begin{pmatrix} 1 & \mathbf{0}_{D_1-1}^T & \mathbf{0}_{D_2-1}^T & \cdots & \mathbf{0}_{D_q-1}^T \\ \mathbf{0}_{D_1-1} & \mathbf{W}_{D_1}^T \mathbf{P}_1 \mathbf{W}_{D_1} & \mathbf{0}_{(D_1-1) \times (D_2-1)} & \cdots & \mathbf{0}_{(D_1-1) \times (D_q-1)} \\ \mathbf{0}_{D_2-1} & \mathbf{0}_{(D_2-1) \times (D_1-1)} & \mathbf{W}_{D_2}^T \mathbf{P}_2 \mathbf{W}_{D_2} & \cdots & \mathbf{0}_{(D_2-1) \times (D_q-1)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \mathbf{0}_{D_q-1} & \mathbf{0}_{(D_q-1) \times (D_1-1)} & \mathbf{0}_{(D_q-1) \times (D_2-1)} & \cdots & \mathbf{W}_{D_q}^T \mathbf{P}_q \mathbf{W}_{D_q} \end{pmatrix}. \quad (\text{C2})$$

According to Property 2.1 (2), $\mathbf{P}$ is an orthogonal matrix. It is clear that we can get the following equations

$$\begin{cases} \mathbf{z}_i^{(\mathbf{P})} = \mathbf{P} \mathbf{z}_i, \\ \mathbf{Z}^{(\mathbf{P})} = \mathbf{Z} \mathbf{P}^T, \\ ((\mathbf{Z}^{(\mathbf{P})})^T \mathbf{Z}^{(\mathbf{P})})^{-1} = ((\mathbf{Z} \mathbf{P}^T)^T \mathbf{Z} \mathbf{P}^T)^{-1} = (\mathbf{P}^T)^{-1} (\mathbf{Z}^T \mathbf{Z})^{-1} \mathbf{P}^{-1} = \mathbf{P} (\mathbf{Z}^T \mathbf{Z})^{-1} \mathbf{P}^T, \\ \hat{\beta}^{(\mathbf{P})} = ((\mathbf{Z}^{(\mathbf{P})})^T \mathbf{Z}^{(\mathbf{P})})^{-1} (\mathbf{Z}^{(\mathbf{P})})^T \mathbf{Y} = \mathbf{P} (\mathbf{Z}^T \mathbf{Z})^{-1} \mathbf{P}^T \mathbf{P} \mathbf{Z}^T \mathbf{Y} = \mathbf{P} (\mathbf{Z}^T \mathbf{Z})^{-1} \mathbf{Z}^T \mathbf{Y} = \mathbf{P} \hat{\beta}, \\ (S^{(\mathbf{P})})^2 = \frac{(\mathbf{Y} - \mathbf{Z}^{(\mathbf{P})} \hat{\beta}^{(\mathbf{P})})^T (\mathbf{Y} - \mathbf{Z}^{(\mathbf{P})} \hat{\beta}^{(\mathbf{P})})}{n - D - 1} = \frac{(\mathbf{Y} - \mathbf{Z} \mathbf{P}^T \mathbf{P} \hat{\beta})^T (\mathbf{Y} - \mathbf{Z} \mathbf{P}^T \mathbf{P} \hat{\beta})}{n - D - 1} = S^2, \end{cases} \quad (\text{C3})$$

where $(S^{(\mathbf{P})})^2$ denotes the unbiased estimator of the residual variance in Equation (C1).

- (1) Without loss of generality, suppose that $j = 1$. If the remaining components of $\mathbf{u}_1$ except for the first component are permuted through permutation matrix $\mathbf{Q}_1$, then

$$\begin{aligned} & \mathbf{W}_{D_1}^T \mathbf{P}_1 \mathbf{W}_{D_1} \\ &= \begin{pmatrix} \sqrt{\frac{D_1-1}{D_1}} & -\frac{1}{\sqrt{D_1(D_1-1)}} \mathbf{j}_{D_1-1}^T \\ \mathbf{0}_{D_1-2} & \mathbf{W}_{D_1-1}^T \end{pmatrix} \begin{pmatrix} 1 & \mathbf{0}_{D_1-1}^T \\ \mathbf{0}_{D_1-1} & \mathbf{Q}_1 \end{pmatrix} \begin{pmatrix} -\frac{\sqrt{\frac{D_1-1}{D_1}}}{\sqrt{D_1(D_1-1)}} \mathbf{j}_{D_1-1} & \mathbf{W}_{D_1-1}^T \end{pmatrix} \\ &= \begin{pmatrix} \frac{D_1-1}{D_1} + \frac{1}{D_1(D_1-1)} \mathbf{j}_{D_1-1}^T \mathbf{Q}_1 \mathbf{j}_{D_1-1} & -\frac{1}{\sqrt{D_1(D_1-1)}} \mathbf{j}_{D_1-1}^T \mathbf{Q}_1 \mathbf{W}_{D_1-1} \\ -\frac{1}{\sqrt{D_1(D_1-1)}} \mathbf{W}_{D_1-1}^T \mathbf{Q}_1 \mathbf{j}_{D_1-1} & \mathbf{W}_{D_1-1}^T \mathbf{Q}_1 \mathbf{W}_{D_1-1} \end{pmatrix} \\ &= \begin{pmatrix} 1 & \mathbf{0}_{D_1-2}^T \\ \mathbf{0}_{D_1-2} & \mathbf{W}_{D_1-1}^T \mathbf{Q}_1 \mathbf{W}_{D_1-1} \end{pmatrix}. \end{aligned} \quad (\text{C4})$$

If the components of $\mathbf{u}_k$ ($k \neq 1$) are permuted through arbitrary permutation matrix $\mathbf{P}_k$ ($k \neq 1$), then the permutation matrix $\mathbf{P}$ in Equation (C2) can be expressed as

$$\mathbf{P} = \begin{pmatrix} 1 & 0 & \mathbf{0}_{D_1-2}^T & \mathbf{0}_{D_2-1}^T & \cdots & \mathbf{0}_{D_q-1}^T \\ 0 & 1 & \mathbf{0}_{D_1-2}^T & \mathbf{0}_{D_2-1}^T & \cdots & \mathbf{0}_{D_q-1}^T \\ \mathbf{0}_{D_1-2} & \mathbf{0}_{D_1-2} & \mathbf{W}_{D_1-1}^T \mathbf{Q}_1 \mathbf{W}_{D_1-1} & \mathbf{0}_{(D_1-2) \times (D_2-1)} & \cdots & \mathbf{0}_{(D_1-2) \times (D_q-1)} \\ \mathbf{0}_{D_2-1} & \mathbf{0}_{D_2-1} & \mathbf{0}_{(D_2-1) \times (D_1-2)} & \mathbf{W}_{D_2}^T \mathbf{P}_2 \mathbf{W}_{D_2} & \cdots & \mathbf{0}_{(D_2-1) \times (D_q-1)} \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \mathbf{0}_{D_q-1} & \mathbf{0}_{D_q-1} & \mathbf{0}_{(D_q-1) \times (D_1-2)} & \mathbf{0}_{(D_q-1) \times (D_2-1)} & \cdots & \mathbf{W}_{D_q}^T \mathbf{P}_q \mathbf{W}_{D_q} \end{pmatrix}. \quad (\text{C5})$$

Put permutation matrix $\mathbf{P}$ in Equation (C5) into Equation (C3), we get $\beta_0 = \beta_0^{(\mathbf{P})}$, $\beta_1 = \beta_1^{(\mathbf{P})}$, and

$$\begin{aligned} \{((\mathbf{Z}^{(\mathbf{P})})^T \mathbf{Z}^{(\mathbf{P})})^{-1}\}_{1,1} &= \mathbf{e}_{D+1,1}^T ((\mathbf{Z}^{(\mathbf{P})})^T \mathbf{Z}^{(\mathbf{P})})^{-1} \mathbf{e}_{D+1,1} = \mathbf{e}_{D+1,1}^T \mathbf{P} (\mathbf{Z}^T \mathbf{Z})^{-1} \mathbf{P}^T \mathbf{e}_{D+1,1} \\ &= \mathbf{e}_{D+1,1}^T (\mathbf{Z}^T \mathbf{Z})^{-1} \mathbf{e}_{D+1,1} = \{(\mathbf{Z}^T \mathbf{Z})^{-1}\}_{1,1}, \end{aligned}$$

$$\begin{aligned} \{((\mathbf{Z}^{(\mathbf{P})})^T \mathbf{Z}^{(\mathbf{P})})^{-1}\}_{2,2} &= \mathbf{e}_{D+1,2}^T ((\mathbf{Z}^{(\mathbf{P})})^T \mathbf{Z}^{(\mathbf{P})})^{-1} \mathbf{e}_{D+1,2} = \mathbf{e}_{D+1,2}^T \mathbf{P} (\mathbf{Z}^T \mathbf{Z})^{-1} \mathbf{P}^T \mathbf{e}_{D+1,2} \\ &= \mathbf{e}_{D+1,2}^T (\mathbf{Z}^T \mathbf{Z})^{-1} \mathbf{e}_{D+1,2} = \{(\mathbf{Z}^T \mathbf{Z})^{-1}\}_{2,2}. \end{aligned}$$

Since $(S^{(\mathbf{P})})^2 = S^2$, the test statistics T_0 and T_1 are invariant.

- (2) If the remaining components of $\mathbf{u}_j$ ($j = 1, 2, \dots, q$) except for the first component are permuted through permutation matrix $\mathbf{Q}_j$, similar to Equation (C4), then the permutation matrix $\mathbf{P}$ in Equation (C2) can be expressed as:

$$\mathbf{P} = \begin{pmatrix} 1 & 0 & \mathbf{0}_{D_1-2}^T & \cdots & 0 & \mathbf{0}_{D_q-2}^T \\ 0 & 1 & \mathbf{0}_{D_1-2}^T & \cdots & 0 & \mathbf{0}_{D_q-2}^T \\ \mathbf{0}_{D_1-2} & \mathbf{0}_{D_1-2} & \mathbf{W}_{D_1-1}^T \mathbf{Q}_1 \mathbf{W}_{D_1-1} & \cdots & \mathbf{0}_{D_1-2} & \mathbf{0}_{(D_1-2) \times (D_q-2)} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \mathbf{0}_{D_1-2}^T & \cdots & 1 & \mathbf{0}_{D_q-2}^T \\ \mathbf{0}_{D_q-2} & \mathbf{0}_{D_q-2} & \mathbf{0}_{(D_q-2) \times (D_1-2)} & \cdots & \mathbf{0}_{D_q-2} & \mathbf{W}_{D_q-1}^T \mathbf{Q}_q \mathbf{W}_{D_q-1} \end{pmatrix}. \quad (\text{C6})$$

It follows from Equation (C3) and Equation (C6) that the parameters β_0, β_{k_j} ($j = 1, 2, \dots, q$) remain unchanged, and

$$\{((\mathbf{Z}^{(\mathbf{P})})^T \mathbf{Z}^{(\mathbf{P})})^{-1}\}_{1,1} = \mathbf{e}_{D+1,1}^T \mathbf{P} (\mathbf{Z}^T \mathbf{Z})^{-1} \mathbf{P}^T \mathbf{e}_{D+1,1} = \{(\mathbf{Z}^T \mathbf{Z})^{-1}\}_{1,1},$$

$$\begin{aligned} \{((\mathbf{Z}^{(\mathbf{P})})^T \mathbf{Z}^{(\mathbf{P})})^{-1}\}_{k_j+1, k_j+1} &= \mathbf{e}_{D+1, k_j+1}^T \mathbf{P} (\mathbf{Z}^T \mathbf{Z})^{-1} \mathbf{P}^T \mathbf{e}_{D+1, k_j+1} \\ &= \mathbf{e}_{D+1, k_j+1}^T (\mathbf{Z}^T \mathbf{Z})^{-1} \mathbf{e}_{D+1, k_j+1} = \{(\mathbf{Z}^T \mathbf{Z})^{-1}\}_{k_j+1, k_j+1}, \end{aligned}$$

where $k_j = \sum_{i=1}^j D_i - D_j - j + 2$ ($j = 1, \dots, q$). Since $(S^{(\mathbf{P})})^2 = S^2$, the test statistics T_0 and T_{k_j} ($j = 1, 2, \dots, q$) are invariant.

- (3) If the components of $\mathbf{u}_j$ ($j = 1, 2, \dots, q$) are permuted through permutation matrix $\mathbf{P}_j$, for convenience, the permutation matrix $\mathbf{P}$ in Equation (C2) is denoted as

$$\mathbf{P} = \begin{pmatrix} 1 & \mathbf{0}_D^T \\ \mathbf{0}_D & \mathbf{Q} \end{pmatrix}, \quad (\text{C7})$$

where $\mathbf{Q}$ is a permutation matrix. Put permutation matrix $\mathbf{P}$ in Equation (C7) into Equation (C3), it is obvious that the test statistic T_0 is invariant. The test statistic

for testing whether all the parameters in Equation (C1) are equal to 0 is

$$\begin{aligned}
& \frac{1}{D(S(\mathbf{P}))^2} (\hat{\boldsymbol{\beta}}_*^{(\mathbf{P})})^T \{((\mathbf{Z}^{(\mathbf{P})})^T \mathbf{Z}^{(\mathbf{P})})^{-1}\}_{-1,-1} \hat{\boldsymbol{\beta}}_*^{(\mathbf{P})} \\
&= \frac{1}{D(S(\mathbf{P}))^2} ((\mathbf{0}_D : \mathbf{I}_D) \hat{\boldsymbol{\beta}}^{(\mathbf{P})})^T (\mathbf{0}_D : \mathbf{I}_D) ((\mathbf{P}^{(\mathbf{P})})^T \mathbf{Z}^{(\mathbf{P})})^{-1} (\mathbf{0}_D : \mathbf{I}_D)^T (\mathbf{0}_D : \mathbf{I}_D) \hat{\boldsymbol{\beta}}^{(\mathbf{P})} \\
&= \frac{1}{D(S(\mathbf{P}))^2} (\hat{\boldsymbol{\beta}}^{(\mathbf{P})})^T \begin{pmatrix} 0 & \mathbf{0}_D^T \\ \mathbf{0}_D & \mathbf{I}_D \end{pmatrix} ((\mathbf{Z}^{(\mathbf{P})})^T \mathbf{Z}^{(\mathbf{P})})^{-1} \begin{pmatrix} 0 & \mathbf{0}_D^T \\ \mathbf{0}_D & \mathbf{I}_D \end{pmatrix} \hat{\boldsymbol{\beta}}^{(\mathbf{P})} \\
&= \frac{1}{D(S(\mathbf{P}))^2} (\hat{\boldsymbol{\beta}})^T \mathbf{P}^T \begin{pmatrix} 0 & \mathbf{0}_D^T \\ \mathbf{0}_D & \mathbf{I}_D \end{pmatrix} \mathbf{P} (\mathbf{Z}^T \mathbf{Z})^{-1} \mathbf{P}^T \begin{pmatrix} 0 & \mathbf{0}_D^T \\ \mathbf{0}_D & \mathbf{I}_D \end{pmatrix} \mathbf{P} \hat{\boldsymbol{\beta}} \\
&= \frac{1}{D(S(\mathbf{P}))^2} (\hat{\boldsymbol{\beta}})^T \begin{pmatrix} 0 & \mathbf{0}_D^T \\ \mathbf{0}_D & \mathbf{I}_D \end{pmatrix} (\mathbf{Z}^T \mathbf{Z})^{-1} \begin{pmatrix} 0 & \mathbf{0}_D^T \\ \mathbf{0}_D & \mathbf{I}_D \end{pmatrix} \hat{\boldsymbol{\beta}} \\
&= \frac{1}{D(S(\mathbf{P}))^2} ((\mathbf{0}_D : \mathbf{I}_D) \hat{\boldsymbol{\beta}})^T (\mathbf{0}_D : \mathbf{I}_D) (\mathbf{Z}^T \mathbf{Z})^{-1} (\mathbf{0}_D : \mathbf{I}_D)^T (\mathbf{0}_D : \mathbf{I}_D) \hat{\boldsymbol{\beta}} \\
&= \frac{1}{DS^2} (\hat{\boldsymbol{\beta}}_*)^T \{(\mathbf{Z}^T \mathbf{Z})^{-1}\}_{-1,-1} \hat{\boldsymbol{\beta}}_*,
\end{aligned}$$

so the test statistic F is invariant under the permutation of $\mathbf{u}_j$.

Appendix D. Proof of Theorem 3.4

According to Property 2.1, Theorem 3.1 and Theorem 3.2, we obtain that

$$\begin{aligned}
\mathbf{c}_0 &= \begin{pmatrix} \mathbf{e}_{L-1,1}^T \mathbf{b}_0^{(1)} \\ \mathbf{e}_{L-1,1}^T \mathbf{b}_0^{(2)} \\ \vdots \\ \mathbf{e}_{L-1,1}^T \mathbf{b}_0^{(L)} \end{pmatrix} = \begin{pmatrix} \mathbf{e}_{L-1,1}^T \mathbf{W}_L^T \mathbf{P}_{L,1} \mathbf{W}_L \mathbf{b}_0 \\ \mathbf{e}_{L-1,1}^T \mathbf{W}_L^T \mathbf{P}_{L,2} \mathbf{W}_L \mathbf{b}_0 \\ \vdots \\ \mathbf{e}_{L-1,1}^T \mathbf{W}_L^T \mathbf{P}_{L,L} \mathbf{W}_L \mathbf{b}_0 \end{pmatrix} = \begin{pmatrix} \mathbf{e}_{L-1,1}^T \mathbf{W}_L^T \mathbf{P}_{L,1} \\ \mathbf{e}_{L-1,1}^T \mathbf{W}_L^T \mathbf{P}_{L,2} \\ \vdots \\ \mathbf{e}_{L-1,1}^T \mathbf{W}_L^T \mathbf{P}_{L,L} \end{pmatrix} \mathbf{W}_L \mathbf{b}_0 \\
&= \sqrt{\frac{L}{L-1}} \mathbf{G}_L \mathbf{W}_L \mathbf{b}_0 = \sqrt{\frac{L}{L-1}} \mathbf{W}_L \mathbf{b}_0 = \sqrt{\frac{L}{L-1}} \text{clr}(\mathbf{a}_0),
\end{aligned}$$

$$\begin{aligned}
\mathbf{C}_j &= \begin{pmatrix} \mathbf{e}_{L-1,1}^T \mathbf{B}_j^{(1,1)} \mathbf{e}_{D_j-1,1} \cdots \mathbf{e}_{L-1,1}^T \mathbf{B}_j^{(1,D_j)} \mathbf{e}_{D_j-1,1} \\ \mathbf{e}_{L-1,1}^T \mathbf{B}_j^{(2,1)} \mathbf{e}_{D_j-1,1} \cdots \mathbf{e}_{L-1,1}^T \mathbf{B}_j^{(2,D_j)} \mathbf{e}_{D_j-1,1} \\ \vdots \quad \quad \quad \ddots \quad \quad \quad \vdots \\ \mathbf{e}_{L-1,1}^T \mathbf{B}_j^{(L,1)} \mathbf{e}_{D_j-1,1} \cdots \mathbf{e}_{L-1,1}^T \mathbf{B}_j^{(L,D_j)} \mathbf{e}_{D_j-1,1} \end{pmatrix} \\
&= \begin{pmatrix} \mathbf{e}_{L-1,1}^T \mathbf{W}_L^T \mathbf{P}_{L,1} \mathbf{W}_L \mathbf{B}_j \mathbf{W}_{D_j}^T (\mathbf{P}_{D_j,1}^T \mathbf{W}_{D_j} \mathbf{e}_{D_j-1,1}, \dots, \mathbf{P}_{D_j,D_j}^T \mathbf{W}_{D_j} \mathbf{e}_{D_j-1,1}) \\ \mathbf{e}_{L-1,1}^T \mathbf{W}_L^T \mathbf{P}_{L,2} \mathbf{W}_L \mathbf{B}_j \mathbf{W}_{D_j}^T (\mathbf{P}_{D_j,1}^T \mathbf{W}_{D_j} \mathbf{e}_{D_j-1,1}, \dots, \mathbf{P}_{D_j,D_j}^T \mathbf{W}_{D_j} \mathbf{e}_{D_j-1,1}) \\ \vdots \\ \mathbf{e}_{L-1,1}^T \mathbf{W}_L^T \mathbf{P}_{L,L} \mathbf{W}_L \mathbf{B}_j \mathbf{W}_{D_j}^T (\mathbf{P}_{D_j,1}^T \mathbf{W}_{D_j} \mathbf{e}_{D_j-1,1}, \dots, \mathbf{P}_{D_j,D_j}^T \mathbf{W}_{D_j} \mathbf{e}_{D_j-1,1}) \end{pmatrix} \\
&= \begin{pmatrix} \mathbf{e}_{L-1,1}^T \mathbf{W}_L^T \mathbf{P}_{L,1} \mathbf{W}_L \mathbf{B}_j \mathbf{W}_{D_j}^T \sqrt{\frac{D_j}{D_j-1}} \mathbf{G}_{D_j} \\ \mathbf{e}_{L-1,1}^T \mathbf{W}_L^T \mathbf{P}_{L,2} \mathbf{W}_L \mathbf{B}_j \mathbf{W}_{D_j}^T \sqrt{\frac{D_j}{D_j-1}} \mathbf{G}_{D_j} \\ \vdots \\ \mathbf{e}_{L-1,1}^T \mathbf{W}_L^T \mathbf{P}_{L,L} \mathbf{W}_L \mathbf{B}_j \mathbf{W}_{D_j}^T \sqrt{\frac{D_j}{D_j-1}} \mathbf{G}_{D_j} \end{pmatrix} \\
&= \sqrt{\frac{D_j}{D_j-1}} \begin{pmatrix} \mathbf{e}_{L-1,1}^T \mathbf{W}_L^T \mathbf{P}_{L,1} \\ \mathbf{e}_{L-1,1}^T \mathbf{W}_L^T \mathbf{P}_{L,2} \\ \vdots \\ \mathbf{e}_{L-1,1}^T \mathbf{W}_L^T \mathbf{P}_{L,L} \end{pmatrix} \mathbf{W}_L \mathbf{B}_j \mathbf{W}_{D_j}^T \mathbf{G}_{D_j} \\
&= \sqrt{\frac{D_j}{D_j-1}} \sqrt{\frac{L}{L-1}} \mathbf{G}_L \mathbf{W}_L \mathbf{B}_j \mathbf{W}_{D_j}^T \mathbf{G}_{D_j} \\
&= \sqrt{\frac{D_j}{D_j-1}} \sqrt{\frac{L}{L-1}} \mathbf{W}_L \mathbf{B}_j \mathbf{W}_{D_j}^T = \sqrt{\frac{D_j}{D_j-1}} \sqrt{\frac{L}{L-1}} \mathbf{A}_j.
\end{aligned}$$

Therefore, $\mathbf{a}_0 = \text{clr}^{-1}(\sqrt{\frac{L-1}{L}} \mathbf{c}_0)$, $\mathbf{A}_j = \sqrt{\frac{L-1}{L}} \sqrt{\frac{D_j-1}{D_j}} \mathbf{C}_j$ ($j = 1, 2, \dots, q$).