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

\[
\begin{align*}
\text{ilr}(u_{ki})(\text{ilr}(v_i))^T &= W_{D_k}^T \log(u_{ki})(\log(v_i))^T W_L, \\
\text{ilr}(u_{ji})(\text{ilr}(u_{ki}))^T &= W_{D_j}^T \log(u_{ji})(\log(u_{ki}))^T W_{D_k}.
\end{align*}
\]

Thus Equation (14) can be deduced to

\[
\begin{align*}
\sum_{i=1}^{n} (\log(v_i))^T W_L \sum_{i=1}^{n} \log(u_{1i})(\log(v_i))^T W_L
\end{align*}
\]

If both sides of Equation (A1) are multiplied from the right-hand side by matrix \(W_L^T\), since \(W_L W_L^T = G_L\), we can get the same solution as Equation (12), so

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\[
\begin{align*}
\begin{cases}
  (\log(a_0))^T G_L = b_0^T W_L^T, \\
  A_j = W_{D_j} B_j^T W_L^T \quad (j = 1, 2, \ldots, q). 
\end{cases}
\end{align*}
\]

\[
\begin{align*}
\begin{cases}
  b_0 = \text{ilr}(a_0), \\
  B_j = W_{D_j}^T A_j W_{D_j} \quad (j = 1, 2, \ldots, q).
\end{cases}
\end{align*}
\] (A2)

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

\[
\text{ilr}(v_i) = \text{ilr}(a_0 \oplus A_1 \boxplus u_{i1} \oplus \cdots \oplus A_q \boxplus u_{qi} \oplus \varepsilon_i)
\]

\[
= \text{ilr}(a_0) + \text{ilr}(A_1 \boxplus u_{i1}) + \cdots + \text{ilr}(A_q \boxplus u_{qi}) + \text{ilr}(\varepsilon_i)
\]

\[
= \text{ilr}(a_0) + W_{D_j}^T A_j \text{ilr}(u_{i1}) + \cdots + W_{D_q}^T A_q \text{ilr}(u_{qi}) + \text{ilr}(\varepsilon_i).
\]

Corresponding to model in Equation (13), we can get the same results with Equation (A2), therefore, \(a_0 = \text{ilr}^{-1}(b_0), \ A_j = W_{L} B_j W_{D_j}^T \quad (j = 1, 2, \ldots, q)\).

**Appendix B. Proof of Theorem 3.2**

For any composition \(v \in S^L\), by Equation (8), we have that

\[
\text{ilr}(v) = W_{L}^T \text{clr}(v) = W_{L}^T \text{clr}(P_{L,0}^T v^{(l_0)}) = W_{L}^T P_{L,0}^T W_{L}^T \text{ilr}(v^{(l_0)}),
\]

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

\[
W_{L}^T P_{L,0}^T W_{L} \text{ilr}(v^{(l_0)}) = b_0 + B_1 W_{D_1}^T P_{D_1,1}^T W_{D_1} \text{ilr}(u_{i1}) + \cdots + B_q W_{D_q}^T P_{D_q,1}^T W_{D_q} \text{ilr}(u_{qi}) + \text{ilr}(\varepsilon_i).
\] (B1)

If both sides of Equation (B1) are multiplied from the left-hand side by matrix \(W_{L}^T P_{L,0}^T W_{L}\), by Property 2.1, we obtain that

\[
\text{ilr}(v_{i1}) = W_{L}^T P_{L,0}^T W_{L} b_0 + W_{L}^T P_{L,0}^T W_{L} B_1 W_{D_1}^T P_{D_1,1}^T W_{D_1} \text{ilr}(u_{i1}) + \cdots
\]

\[
+ W_{L}^T P_{L,0}^T W_{L} B_q W_{D_q}^T P_{D_q,1}^T W_{D_q} \text{ilr}(u_{qi}) + W_{L}^T P_{L,0}^T W_{L} \text{ilr}(\varepsilon_i).
\]

Compared with model in Equation (15), it is clear that \(b_0^{(l_0)} = W_{L}^T P_{L,0}^T W_{L} b_0, \ B_j^{(l_j,1)} = W_{L}^T P_{L,0}^T W_{L} B_j W_{D_j}^T P_{D_j,1}^T W_{D_j} (j = 1, 2, \ldots, q)\).

**Appendix C. Proof of Theorem 3.3**

Without loss of generality, suppose that \(l_0 = l_1 = \cdots = l_q = 1\), the model in Equation (17) is simplified to \(E(Y|Z) = Z \beta\). When composition \(u_j \quad (j = 1, 2, \cdots, q)\) is permuted through a \(D_j \times D_j\) permutation matrix \(P_j\), we get the regression equation

\[
E(Y|Z^{(P)}) = Z^{(P)} \beta^{(P)},
\] (C1)
where $Z^{(P)} = (z_1^{(P)}, z_2^{(P)}, \ldots, z_n^{(P)})^T$, $z_i^{(P)} = (1, (\text{irr}(P_1 u_{1i})))^T, (\text{irr}(P_2 u_{2i})))^T, \ldots, (\text{irr}(P_q u_{qi})))^T$, $\beta^{(P)}$ is the regression coefficient vector. By Equation (8), we have

$$\text{irr}(P_j u_{ji}) = W_{D_j}^T \text{clr}(P_j u_{ji}) = W_{D_j}^T P_j \text{clr}(u_{ji}) = W_{D_j}^T P_j W_D \text{irr}(u_{ji}),$$

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

$$P = \begin{pmatrix}
1 & 0_{D_1-1}^T & 0_{D_2-1}^T & \cdots & 0_{D_{n-1}}^T \\
0_{D_1-1} & W_{D_1}^T P_1 W_{D_1} & 0_{(D_1-1) \times (D_1-1)} & \cdots & 0_{(D_1-1) \times (D_{n-1})} \\
0_{D_2-1} & 0_{(D_2-1) \times (D_1-1)} & W_{D_2}^T P_2 W_{D_2} & \cdots & 0_{(D_2-1) \times (D_{n-1})} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
0_{D_{n-1}} & 0_{(D_{n-1}) \times (D_1-1)} & 0_{(D_{n-1}) \times (D_2-1)} & \cdots & W_{D_{n-1}}^T P_q W_{D_{n-1}}
\end{pmatrix}. \quad (C2)$$

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

$$\begin{align*}
(z_i^{(P)})^T P & = z_i, \\
Z^{(P)} & = ZP^T, \\
((Z^{(P)})^T Z^{(P)})^{-1} & = ((Z P^T Z P^T)^{-1} = (P^T)^{-1} (Z^T Z)^{-1} P^T = P (Z^T Z)^{-1} P^T, \\
\hat{\beta}^{(P)} & = ((Z^{(P)})^T Z^{(P)})^{-1} (Z^{(P)})^T P Z^{(P)} = P (Z^T Z)^{-1} P^T Y = P \hat{\beta}, \\
(S^{(P)})^2 & = \frac{(Y - Z \hat{\beta}^{(P)})^T (Y - Z \hat{\beta}^{(P)})}{n - D - 1} = \frac{(Y - Z \hat{\beta}^{T} P \hat{\beta}^{(P)})^T (Y - Z \hat{\beta}^{T} P \hat{\beta})}{n - D - 1} = S^2, \quad (C3)
\end{align*}$$

where $(S^{(P)})^2$ 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 $u_1$ except for the first component are permuted through permutation matrix $Q_1$, then

$$W_{D_1}^T P_1 W_{D_1},$$

$$\begin{align*}
& = \left(\sqrt{\frac{D_1}{D_1-1}} - \sqrt{\frac{1}{D_1(D_1-1)}} j_{D_1-1}^T \right) \begin{pmatrix} 1 & 0_{D_1-1}^T & 0_{D_2-1}^T & \cdots & 0_{D_{n-1}}^T \\
0_{D_1-1} & W_{D_1}^T & 0_{(D_1-1) \times (D_1-1)} & \cdots & 0_{(D_1-1) \times (D_{n-1})} \\
0_{D_2-1} & 0_{(D_2-1) \times (D_1-1)} & W_{D_2}^T & \cdots & 0_{(D_2-1) \times (D_{n-1})} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
0_{D_{n-1}} & 0_{(D_{n-1}) \times (D_1-1)} & 0_{(D_{n-1}) \times (D_2-1)} & \cdots & W_{D_{n-1}}^T \\
\end{pmatrix} Q_1 W_{D_1} \\
& = \begin{pmatrix} \frac{D_1}{D_1-1} + \frac{1}{\sqrt{D_1(D_1-1)}} j_{D_1-1}^T & 0_{D_1-1}^T & 0_{D_2-1}^T & \cdots & 0_{D_{n-1}}^T \\
-\frac{1}{\sqrt{D_1(D_1-1)}} j_{D_1-1}^T & W_{D_1}^T & 0_{(D_1-1) \times (D_2-1)} & \cdots & 0_{(D_1-1) \times (D_{n-1})} \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
0_{D_{n-1}} & 0_{(D_{n-1}) \times (D_2-1)} & 0_{(D_{n-1}) \times (D_{n-1})} & \cdots & W_{D_{n-1}}^T \\
\end{pmatrix} Q_1 W_{D_1} \\
& = \begin{pmatrix} 1 & 0_{D_1-2}^T \end{pmatrix} W_{D_1}^T Q_1 W_{D_1}. \quad (C4)
\end{align*}$$

If the components of $u_k$ ($k \neq 1$) are permuted through arbitrary permutation matrix $P_k$ ($k \neq 1$), then the permutation matrix $P$ in Equation (C2) can be expressed as

$$P = \begin{pmatrix}
1 & 0_{D_1-2}^T & 0_{D_2-1}^T & \cdots & 0_{D_{n-1}}^T \\
0 & 1 & 0_{D_1-2}^T & \cdots & 0_{D_{n-1}}^T \\
0_{D_1-2} & 0_{D_1-2} & W_{D_1-1} & 0_{(D_1-2) \times (D_1-1)} & \cdots & 0_{(D_1-2) \times (D_{n-1})} \\
0_{D_2-1} & 0_{(D_2-1) \times (D_1-1)} & W_{D_2} & 0_{(D_2-1) \times (D_{n-1})} & \cdots & 0_{(D_2-1) \times (D_{n-1})} \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0_{D_{n-1}} & 0_{D_{n-1}} & 0_{(D_{n-1}) \times (D_1-2)} & 0_{(D_{n-1}) \times (D_2-1)} & \cdots & W_{D_{n-1}}^T P_q W_{D_{n-1}}
\end{pmatrix}. \quad (C5)
Put permutation matrix $\mathbf{P}$ in Equation (C5) into Equation (C3), we get $\beta_0 = \beta_0^{(P)}$, $\beta_1 = \beta_1^{(P)}$, and

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

$$\{(Z^{(P)})^T Z^{(P)}\}^{-1}_{2,2} = e_{D+1,2}^T (Z^{(P)})^T Z^{(P)} e_{D+1,2} = e_{D+1,2}^T P (Z^T Z)^{-1} P^T e_{D+1,2} = e_{D+1,2}^T (Z^T Z)^{-1} e_{D+1,2} = \{(Z^T Z)^{-1}\}_{2,2}.$$

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

(2) If the remaining components of $\mathbf{u}_j (j = 1, 2, \cdots, q)$ 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:

$$\mathbf{P} = \begin{pmatrix} 1 & 0 & 0_{D_1-2} & \cdots & 0_{D_n-2} \\ 0 & 1 & 0_{D_1-2} & \cdots & 0_{D_n-2} \\ 0_{D_1-2} & 0_{D_2-2} & \mathbf{W}_{D_1-1}^T \mathbf{Q}_1 \mathbf{W}_{D_2-1} \cdots & 0_{D_1-2} & 0_{(D_1-2) \times (D_1-2)} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0_{D_2-2} & \cdots & 1_{D_2-2} \\ 0_{D_1-2} & 0_{D_2-2} & \mathbf{W}_{D_1-1}^T \mathbf{Q}_2 \mathbf{W}_{D_2-1} \cdots & 0_{D_1-2} & \mathbf{W}_{D_2-2} \end{pmatrix}. \quad (C6)$$

It follows from Equation (C3) and Equation (C6) that the parameters $\beta_0, \beta_k, (j = 1, 2, \cdots, q)$ remain unchanged, and

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

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

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

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

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

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
According to Property 2.1, Theorem 3.1 and Theorem 3.2, we obtain that for testing whether all the parameters in Equation (C1) are equal to 0 is

\[
\frac{1}{D(S(P))^2} \hat{\beta}^{(P)} T \{ ((Z(P))^T Z(P))^{-1} \}_{-1,-1} \hat{\beta}^{(P)}
\]

\[
= \frac{1}{D(S(P))^2} ((0_D : I_D) \hat{\beta}^{(P)} (0_D : I_D)((P(P))^T Z(P))^{-1} (0_D : I_D)^T (0_D : I_D) \hat{\beta}^{(P)}
\]

\[
= \frac{1}{D(S(P))^2} (\hat{\beta}^{(P)} T\left( \begin{array}{cc} 0 & 0^T_D \\ 0_D & I_D \end{array} \right) (Z(P))^T Z(P))^{-1} (0_D : I_D)^T \hat{\beta}
\]

\[
= \frac{1}{D(S(P))^2} (\hat{\beta}^{(P)} T\left( \begin{array}{cc} 0 & 0^T_D \\ 0_D & I_D \end{array} \right) (Z)^T Z)^{-1} (0_D : I_D)^T \hat{\beta}
\]

so the test statistic \( F \) is invariant under the permutation of \( u_j \).

Appendix D. Proof of Theorem 3.4

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

\[
c_0 = \left( \begin{array}{c} e_{L-1,1}^T b_0^{(1)} \\ e_{L-1,1}^T b_0^{(2)} \\ \vdots \\ e_{L-1,1}^T b_0^{(L)} \end{array} \right) = \left( \begin{array}{c} e_{L-1,1}^T W_L^T P_L,1 W_L b_0 \\ e_{L-1,1}^T W_L^T P_L,2 W_L b_0 \\ \vdots \\ e_{L-1,1}^T W_L^T P_L,L W_L b_0 \end{array} \right) = \left( \begin{array}{c} e_{L-1,1}^T W_L^T P_L,1 \\ e_{L-1,1}^T W_L^T P_L,2 \\ \vdots \\ e_{L-1,1}^T W_L^T P_L,L \end{array} \right) W_L b_0
\]

\[
= \sqrt{\frac{L}{L-1}} G_L W_L b_0 = \sqrt{\frac{L}{L-1}} W_L b_0 = \sqrt{\frac{L}{L-1}} \text{clr}(a_0),
\]
Therefore, 

\[ \mathbf{a}_0 = \text{clr}^{-1}(\sqrt{\frac{L-1}{L}} \mathbf{c}_0), \quad \mathbf{A}_j = \sqrt{\frac{L-1}{L}} \mathbf{D}_j \mathbf{C}_j \quad (j = 1, 2, \ldots, q). \]