

## PROOF OF BÖTTCHER AND WENZEL'S CONJECTURE

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*Abstract.* In 2005, Böttcher and Wenzel raised a conjecture that if  $X$  and  $Y$  are any two real  $n$ -by- $n$  matrices, then  $\|XY - YX\|_F^2 \leq 2\|X\|_F^2\|Y\|_F^2$ , where  $\|\cdot\|_F$  denotes the Frobenius norm. They proved this for the case of 2-by-2 matrices. Later, László proved the conjecture for the case of 3-by-3 matrices. In this paper, we prove the conjecture for general  $n$ -by- $n$  matrices.

### 1. Introduction

Böttcher and Wenzel proposed the following conjecture in [1]: the upper bound of the Frobenius norm of the commutator of any two  $n$ -by- $n$  real matrices  $X$  and  $Y$  is given by

$$\|XY - YX\|_F^2 \leq 2\|X\|_F^2\|Y\|_F^2.$$

They also proved that the inequality is true for the case of  $n = 2$ . Very recently, László [3] proved the conjecture for the case of  $n = 3$ . In this paper, we prove the conjecture for general  $n$ . In next section, for simplicity, we will give a detailed proof of the conjecture for the case of  $n = 3$ . An outline of the proof for general  $n$  can be found in Section 3. We emphasize that our proof for the case of  $n = 3$  is completely different from that provided in [3]. As to our knowledge, the technique of [3] cannot be applied to prove the conjecture in the general case.

### 2. The proof

Our analysis will show that the conjecture has close connection with the Cauchy-Schwarz inequality [2]. To get a sharper bound, the difference between the two sides of the Cauchy-Schwarz inequality has to be taken into account. The following Lagrange

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identity [3] serves this purpose:

$$\begin{aligned} \left(\sum_{i=1}^n \alpha_i \beta_i\right)^2 &= \sum_{i=1}^n \alpha_i^2 \sum_{i=1}^n \beta_i^2 - \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n (\alpha_i \beta_j - \alpha_j \beta_i)^2 \\ &= \sum_{i=1}^n \alpha_i^2 \sum_{i=1}^n \beta_i^2 - \sum_{i=1}^n \sum_{j>i} \left| \begin{matrix} \alpha_i & \alpha_j \\ \beta_i & \beta_j \end{matrix} \right|^2. \end{aligned}$$

It will be used repeatedly throughout our analysis.

For  $n = 3$ , let  $X = USV$  be the singular value decomposition of  $X$  where  $S \equiv \text{diag}(s_1, s_2, s_3)$  and  $U, V$  are (real) orthogonal. Denote

$$B \equiv VYV^T \equiv [b_{ij}]_{i,j=1}^3, \quad Q \equiv VU, \quad C \equiv Q^T BQ \equiv [c_{ij}]_{i,j=1}^3.$$

Note that  $Q$  is also orthogonal. By the Cauchy-Schwarz inequality,

$$\begin{aligned} \|XY - YX\|_F^2 &= \|USVY - YUSV\|_F^2 = \|SB - CS\|_F^2 \\ &= (s_1 b_{11} - s_1 c_{11})^2 + (s_1 b_{12} - s_2 c_{12})^2 + (s_1 b_{13} - s_3 c_{13})^2 \\ &\quad + (s_2 b_{21} - s_1 c_{21})^2 + (s_2 b_{22} - s_2 c_{22})^2 + (s_2 b_{23} - s_3 c_{23})^2 \\ &\quad + (s_3 b_{31} - s_1 c_{31})^2 + (s_3 b_{32} - s_2 c_{32})^2 + (s_3 b_{33} - s_3 c_{33})^2 \\ &\leq (s_1^2 b_{11}^2 + s_1^2 c_{11}^2 - 2s_1^2 b_{11}c_{11}) + (s_1^2 + s_2^2)(b_{12}^2 + c_{12}^2) \\ &\quad + (s_1^2 + s_3^2)(b_{13}^2 + c_{13}^2) + (s_2^2 + s_1^2)(b_{21}^2 + c_{21}^2) \\ &\quad + (s_2^2 b_{22}^2 + s_2^2 c_{22}^2 - 2s_2^2 b_{22}c_{22}) + (s_2^2 + s_3^2)(b_{23}^2 + c_{23}^2) \\ &\quad + (s_3^2 + s_1^2)(b_{31}^2 + c_{31}^2) + (s_3^2 + s_2^2)(b_{32}^2 + c_{32}^2) \\ &\quad + (s_3^2 b_{33}^2 + s_3^2 c_{33}^2 - 2s_3^2 b_{33}c_{33}) \\ &= \sum_{j=1}^3 s_j^2 \Delta_j, \end{aligned}$$

where

$$\Delta_j \equiv b_{jj}^2 + c_{jj}^2 - 2b_{jj}c_{jj} + \sum_{k \neq j} b_{jk}^2 + \sum_{k \neq j} c_{kj}^2 + \sum_{k \neq j} c_{jk}^2 + \sum_{k \neq j} b_{kj}^2, \tag{1}$$

for  $j = 1, 2, 3$ . The conjecture follows if we can prove that

$$\Delta_j \leq 2\|B\|_F^2, \quad j = 1, 2, 3.$$

The rest of the proof will concentrate on this claim. Without loss of generality, we only carry out our analysis on  $\Delta_1$ .

Let  $\mathbf{q} \equiv (q_1, q_2, q_3)$  be the first row of  $Q^T$  and  $\mathbf{r}_i$  be the  $i$ -th row of  $B$ , i.e.,

$$B \equiv [b_{ij}]_{i,j=1}^3 = \begin{bmatrix} \mathbf{r}_1 \\ \mathbf{r}_2 \\ \mathbf{r}_3 \end{bmatrix}.$$

Then we have by the fact that  $Q$  is (real) orthogonal,

$$\begin{aligned} \sum_{k=1}^3 c_{1k}^2 &= \|\mathbf{q}BQ\|_2^2 = \|\mathbf{q}B\|_2^2 \\ &= q_1^2\|\mathbf{r}_1\|_2^2 + q_2^2\|\mathbf{r}_2\|_2^2 + q_3^2\|\mathbf{r}_3\|_2^2 + 2q_1q_2\mathbf{r}_1 \cdot \mathbf{r}_2^T + 2q_1q_3\mathbf{r}_1 \cdot \mathbf{r}_3^T + 2q_2q_3\mathbf{r}_2 \cdot \mathbf{r}_3^T, \end{aligned}$$

and

$$\sum_{k=1}^3 c_{k1}^2 = \|(Q^T B \mathbf{q}^T)^T\|_2^2 = \|\mathbf{q}B^T\|_2^2 = (\mathbf{q} \cdot \mathbf{r}_1^T)^2 + (\mathbf{q} \cdot \mathbf{r}_2^T)^2 + (\mathbf{q} \cdot \mathbf{r}_3^T)^2. \quad (2)$$

On the other hand, since

$$c_{11} = \mathbf{q} \cdot (\mathbf{r}_1 \cdot \mathbf{q}^T, \mathbf{r}_2 \cdot \mathbf{q}^T, \mathbf{r}_3 \cdot \mathbf{q}^T)^T,$$

we have by using the Lagrange identity and  $\|\mathbf{q}\|_2 = 1$ ,

$$\begin{aligned} c_{11}^2 &= \|\mathbf{q}\|_2^2 \left[ (\mathbf{r}_1 \cdot \mathbf{q}^T)^2 + (\mathbf{r}_2 \cdot \mathbf{q}^T)^2 + (\mathbf{r}_3 \cdot \mathbf{q}^T)^2 \right] \\ &\quad - \left| \begin{array}{cc} q_1 & q_2 \\ \mathbf{r}_1 \cdot \mathbf{q}^T & \mathbf{r}_2 \cdot \mathbf{q}^T \end{array} \right|^2 - \left| \begin{array}{cc} q_1 & q_3 \\ \mathbf{r}_1 \cdot \mathbf{q}^T & \mathbf{r}_3 \cdot \mathbf{q}^T \end{array} \right|^2 - \left| \begin{array}{cc} q_2 & q_3 \\ \mathbf{r}_2 \cdot \mathbf{q}^T & \mathbf{r}_3 \cdot \mathbf{q}^T \end{array} \right|^2 \\ &= (\mathbf{q} \cdot \mathbf{r}_1^T)^2 + (\mathbf{q} \cdot \mathbf{r}_2^T)^2 + (\mathbf{q} \cdot \mathbf{r}_3^T)^2 - I_{12} - I_{13} - I_{23}, \end{aligned} \quad (3)$$

where

$$I_{12} \equiv \left| \begin{array}{cc} q_1 & q_2 \\ \mathbf{r}_1 \cdot \mathbf{q}^T & \mathbf{r}_2 \cdot \mathbf{q}^T \end{array} \right|^2, \quad I_{13} \equiv \left| \begin{array}{cc} q_1 & q_3 \\ \mathbf{r}_1 \cdot \mathbf{q}^T & \mathbf{r}_3 \cdot \mathbf{q}^T \end{array} \right|^2, \quad I_{23} \equiv \left| \begin{array}{cc} q_2 & q_3 \\ \mathbf{r}_2 \cdot \mathbf{q}^T & \mathbf{r}_3 \cdot \mathbf{q}^T \end{array} \right|^2.$$

Substituting (3) into (2), we obtain

$$c_{21}^2 + c_{31}^2 = I_{12} + I_{13} + I_{23}.$$

Thus for  $j = 1$ , (1) can be rewritten as

$$\begin{aligned} \Delta_1 &= \|B\|_F^2 - b_{22}^2 - b_{33}^2 - b_{32}^2 - b_{23}^2 - 2\left[\mathbf{q} \cdot (\mathbf{r}_1 \cdot \mathbf{q}^T, \mathbf{r}_2 \cdot \mathbf{q}^T, \mathbf{r}_3 \cdot \mathbf{q}^T)^T\right] b_{11} \\ &\quad + q_1^2\|\mathbf{r}_1\|_2^2 + q_2^2\|\mathbf{r}_2\|_2^2 + q_3^2\|\mathbf{r}_3\|_2^2 + 2q_1q_2\mathbf{r}_1 \cdot \mathbf{r}_2^T + 2q_1q_3\mathbf{r}_1 \cdot \mathbf{r}_3^T + 2q_2q_3\mathbf{r}_2 \cdot \mathbf{r}_3^T \\ &\quad + I_{12} + I_{13} + I_{23}. \end{aligned} \quad (4)$$

Now notice that the sum of the terms coming from  $c_{ij}^2$  must be less than  $\|B\|_F^2$ . To find the difference between them, the Lagrange identity comes into play again. More

precisely, we have

$$\begin{aligned}
 & 2q_1q_2\mathbf{r}_1 \cdot \mathbf{r}_2^T + I_{12} \\
 &= 2q_1q_2\mathbf{r}_1 \cdot \mathbf{r}_2^T + [q_1(q_1b_{21} - q_2b_{11}) + q_2(q_1b_{22} - q_2b_{12}) + q_3(q_1b_{23} - q_2b_{13})]^2 \\
 &\leq 2q_1q_2\mathbf{r}_1 \cdot \mathbf{r}_2^T + \|\mathbf{q}\|_2^2 \left[ (q_1b_{21} - q_2b_{11})^2 + (q_1b_{22} - q_2b_{12})^2 + (q_1b_{23} - q_2b_{13})^2 \right] \\
 &\quad - \left| \begin{matrix} q_1 & q_2 \\ (q_1b_{21} - q_2b_{11}) & (q_1b_{22} - q_2b_{12}) \end{matrix} \right|^2 - \left| \begin{matrix} q_1 & q_3 \\ (q_1b_{21} - q_2b_{11}) & (q_1b_{23} - q_2b_{13}) \end{matrix} \right|^2 \\
 &= q_1^2\|\mathbf{r}_2\|_2^2 + q_2^2\|\mathbf{r}_1\|_2^2 - J_{12,2} - J_{12,3}
 \end{aligned}$$

with

$$\begin{aligned}
 J_{12,2} &\equiv \left| \begin{matrix} q_1 & q_2 \\ (q_1b_{21} - q_2b_{11}) & (q_1b_{22} - q_2b_{12}) \end{matrix} \right|^2, \\
 J_{12,3} &\equiv \left| \begin{matrix} q_1 & q_3 \\ (q_1b_{21} - q_2b_{11}) & (q_1b_{23} - q_2b_{13}) \end{matrix} \right|^2;
 \end{aligned}$$

$$\begin{aligned}
 & 2q_1q_3\mathbf{r}_1 \cdot \mathbf{r}_3^T + I_{13} \\
 &= 2q_1q_3\mathbf{r}_1 \cdot \mathbf{r}_3^T + [q_1(q_1b_{31} - q_3b_{11}) + q_2(q_1b_{32} - q_3b_{12}) + q_3(q_1b_{33} - q_3b_{13})]^2 \\
 &\leq 2q_1q_3\mathbf{r}_1 \cdot \mathbf{r}_3^T + \|\mathbf{q}\|_2^2 \left[ (q_1b_{31} - q_3b_{11})^2 + (q_1b_{32} - q_3b_{12})^2 + (q_1b_{33} - q_3b_{13})^2 \right] \\
 &\quad - \left| \begin{matrix} q_1 & q_2 \\ (q_1b_{31} - q_3b_{11}) & (q_1b_{32} - q_3b_{12}) \end{matrix} \right|^2 - \left| \begin{matrix} q_1 & q_3 \\ (q_1b_{31} - q_3b_{11}) & (q_1b_{33} - q_3b_{13}) \end{matrix} \right|^2 \\
 &= q_1^2\|\mathbf{r}_3\|_2^2 + q_3^2\|\mathbf{r}_1\|_2^2 - J_{13,2} - J_{13,3}
 \end{aligned}$$

with

$$\begin{aligned}
 J_{13,2} &\equiv \left| \begin{matrix} q_1 & q_2 \\ (q_1b_{31} - q_3b_{11}) & (q_1b_{32} - q_3b_{12}) \end{matrix} \right|^2, \\
 J_{13,3} &\equiv \left| \begin{matrix} q_1 & q_3 \\ (q_1b_{31} - q_3b_{11}) & (q_1b_{33} - q_3b_{13}) \end{matrix} \right|^2;
 \end{aligned}$$

and similarly

$$2q_2q_3\mathbf{r}_2 \cdot \mathbf{r}_3^T + I_{23} \leq q_3^2\|\mathbf{r}_2\|_2^2 + q_2^2\|\mathbf{r}_3\|_2^2.$$

Putting all these inequalities into (4), we get

$$\begin{aligned}
 \Delta_1 &\leq 2\|B\|_F^2 - b_{22}^2 - b_{33}^2 - b_{32}^2 - b_{23}^2 - 2q_1^2b_{11}^2 - 2q_2^2b_{11}b_{22} - 2q_3^2b_{11}b_{33} \\
 &\quad - 2q_2q_3(b_{23} + b_{32})b_{11} - 2q_1q_2(b_{12} + b_{21})b_{11} - 2q_1q_3(b_{13} + b_{31})b_{11} \quad (5) \\
 &\quad - J_{12,2} - J_{12,3} - J_{13,2} - J_{13,3}.
 \end{aligned}$$

We must find negative terms to dominate  $-2q_1q_2(b_{12} + b_{21})b_{11} - 2q_1q_3(b_{13} + b_{31})b_{11}$  and those terms, in fact, can be absorbed in the “ $J$ ” terms. However, it is not trivial to estimate the proportion to which these terms should be associated to the “ $J$ ” terms although it turns out to be quite intuitive.

We first notice that  $\Delta_1 \leq 2\|B\|_F^2$  obviously holds when  $q_1^2 = 1$  (i.e.,  $q_2 = q_3 = 0$ ). Therefore, in the following, we assume that  $q_1^2 \neq 1$  and denote  $M^2 \equiv q_2^2 + q_3^2 > 0$ . We have

$$\begin{aligned}
& -J_{12,2} - 2q_1q_2\frac{q_2^2}{M^2}(b_{12} + b_{21})b_{11} \\
& = -q_2^4b_{11}^2 - (q_1q_2b_{21} + q_1q_2b_{12} - q_1^2b_{22})^2 + 2q_2^2b_{11}(q_1q_2b_{21} + q_1q_2b_{12} - q_1^2b_{22}) \\
& \quad - 2q_1q_2\frac{q_2^2}{M^2}(b_{12} + b_{21})b_{11} + 2q_2^2\frac{q_1^2}{M^2}b_{11}b_{22} - 2q_2^2\frac{q_1^2}{M^2}b_{11}b_{22} \\
& = -\left[q_1q_2b_{21} + q_1q_2b_{12} - q_1^2b_{22} - \frac{(M^2-1)}{M^2}q_2^2b_{11}\right]^2 \\
& \quad + \frac{q_1^4}{M^4}q_2^4b_{11}^2 - q_2^4b_{11}^2 - 2q_2^2\frac{q_1^2}{M^2}b_{11}b_{22}; \\
& -J_{13,3} - 2q_1q_3\frac{q_3^2}{M^2}(b_{13} + b_{31})b_{11} \\
& = -q_3^4b_{11}^2 - (q_1q_3b_{31} + q_1q_3b_{13} - q_1^2b_{33})^2 + 2q_3^2b_{11}(q_1q_3b_{31} + q_1q_3b_{13} - q_1^2b_{33}) \\
& \quad - 2q_1q_3\frac{q_3^2}{M^2}(b_{13} + b_{31})b_{11} + 2q_3^2\frac{q_1^2}{M^2}b_{11}b_{33} - 2q_3^2\frac{q_1^2}{M^2}b_{11}b_{33} \\
& = -\left[q_1q_3b_{31} + q_1q_3b_{13} - q_1^2b_{33} - \frac{(M^2-1)}{M^2}q_3^2b_{11}\right]^2 \\
& \quad + \frac{q_1^4}{M^4}q_3^4b_{11}^2 - q_3^4b_{11}^2 - 2q_3^2\frac{q_1^2}{M^2}b_{11}b_{33}; \\
& -J_{12,3} - 2q_2q_3\frac{q_1}{M^2}(q_3b_{21} + q_2b_{13})b_{11} \\
& = -q_2^2q_3^2b_{11}^2 - (q_1q_3b_{21} + q_1q_2b_{13} - q_1^2b_{23})^2 + 2q_2q_3b_{11}(q_1q_3b_{21} + q_1q_2b_{13} - q_1^2b_{23}) \\
& \quad - 2q_2q_3\frac{q_1}{M^2}(q_3b_{21} + q_2b_{13})b_{11} + 2q_2q_3\frac{q_1^2}{M^2}b_{11}b_{23} - 2q_2q_3\frac{q_1^2}{M^2}b_{11}b_{23} \\
& = -\left[q_1q_3b_{21} + q_1q_2b_{13} - q_1^2b_{23} - \frac{(M^2-1)}{M^2}q_2q_3b_{11}\right]^2 \\
& \quad + \frac{q_1^4}{M^4}q_2^2q_3^2b_{11}^2 - q_2^2q_3^2b_{11}^2 - 2q_2q_3\frac{q_1^2}{M^2}b_{11}b_{23};
\end{aligned}$$

and

$$\begin{aligned}
& -J_{13,2} - 2q_2q_3\frac{q_1}{M^2}(q_2b_{31} + q_3b_{12})b_{11} \\
& = -q_2^2q_3^2b_{11}^2 - (q_1q_2b_{31} + q_1q_3b_{12} - q_1^2b_{32})^2 + 2q_2q_3b_{11}(q_1q_2b_{31} + q_1q_3b_{12} - q_1^2b_{32}) \\
& \quad - 2q_2q_3\frac{q_1}{M^2}(q_2b_{31} + q_3b_{12})b_{11} + 2q_2q_3\frac{q_1^2}{M^2}b_{11}b_{32} - 2q_2q_3\frac{q_1^2}{M^2}b_{11}b_{32} \\
& = -\left[q_1q_2b_{31} + q_1q_3b_{12} - q_1^2b_{32} - \frac{(M^2-1)}{M^2}q_2q_3b_{11}\right]^2 \\
& \quad + \frac{q_1^4}{M^4}q_2^2q_3^2b_{11}^2 - q_2^2q_3^2b_{11}^2 - 2q_2q_3\frac{q_1^2}{M^2}b_{11}b_{32}.
\end{aligned}$$

It is easy to see that

$$\begin{aligned}
& 2q_1q_2\frac{q_2^2}{M^2}(b_{12} + b_{21})b_{11} + 2q_1q_3\frac{q_3^2}{M^2}(b_{13} + b_{31})b_{11} \\
& \quad + 2q_2q_3\frac{q_1}{M^2}(q_3b_{21} + q_2b_{13})b_{11} + 2q_2q_3\frac{q_1}{M^2}(q_2b_{31} + q_3b_{12})b_{11} \\
& = 2q_1q_2(b_{12} + b_{21})b_{11} + 2q_1q_3(b_{13} + b_{31})b_{11}.
\end{aligned}$$

Substituting all these into (5), we finally obtain

$$\begin{aligned}
\Delta_1 &\leq 2\|B\|_F^2 - b_{22}^2 - b_{33}^2 - b_{32}^2 - b_{23}^2 - 2q_1^2 b_{11}^2 - 2q_2^2 b_{11} b_{22} - 2q_3^2 b_{11} b_{33} \\
&\quad - 2q_2 q_3 b_{23} b_{11} - 2q_2 q_3 b_{32} b_{11} + \frac{q_1^4}{M^4} q_2^4 b_{11}^2 - q_2^4 b_{11}^2 - 2q_2^2 \frac{q_1^2}{M^2} b_{11} b_{22} + \frac{q_1^4}{M^4} q_3^4 b_{11}^2 \\
&\quad - q_3^4 b_{11}^2 - 2q_3^2 \frac{q_1^2}{M^2} b_{11} b_{33} + \frac{q_1^4}{M^4} q_2^2 q_3^2 b_{11}^2 - q_2^2 q_3^2 b_{11}^2 - 2q_2 q_3 \frac{q_1^2}{M^2} b_{11} b_{23} + \frac{q_1^4}{M^4} q_2^2 q_3^2 b_{11}^2 \\
&\quad - q_2^2 q_3^2 b_{11}^2 - 2q_2 q_3 \frac{q_1^2}{M^2} b_{11} b_{32} \\
&= 2\|B\|_F^2 - b_{22}^2 - b_{33}^2 - b_{32}^2 - b_{23}^2 + \left[ \left( \frac{q_1^4}{M^4} - 1 \right) (q_2^2 + q_3^2)^2 - 2q_1^2 \right] b_{11}^2 \\
&\quad - 2q_2^2 \left( 1 + \frac{q_1^2}{M^2} \right) b_{11} b_{22} - 2q_3^2 \left( 1 + \frac{q_1^2}{M^2} \right) b_{11} b_{33} - 2q_2 q_3 \left( 1 + \frac{q_1^2}{M^2} \right) (b_{23} + b_{32}) b_{11} \\
&= 2\|B\|_F^2 - b_{22}^2 - b_{33}^2 - b_{32}^2 - b_{23}^2 + [(1 - M^2)^2 - M^4 - 2(1 - M^2)] b_{11}^2 \\
&\quad - \frac{2}{M^2} [q_2^2 b_{22} + q_3^2 b_{33} + q_2 q_3 (b_{23} + b_{32})] b_{11} \\
&\leq 2\|B\|_F^2 - b_{11}^2 + \frac{1}{M^4} (q_2^4 + q_3^4 + 2q_2^2 q_3^2) b_{11}^2 = 2\|B\|_F^2.
\end{aligned}$$

### 3. Outline of the proof for general $n$

We are going to give an outline of the proof of the conjecture for general  $n$ . Denote

$$B \equiv VYV^T \equiv [b_{ij}]_{i,j=1}^n, \quad Q \equiv VU, \quad C \equiv Q^T BQ \equiv [c_{ij}]_{i,j=1}^n.$$

For  $n \geq 3$ , we have similarly,

$$\|XY - YX\|_F^2 \leq \sum_{j=1}^n s_j^2 \Delta_j,$$

where

$$\Delta_j = b_{jj}^2 + c_{jj}^2 - 2b_{jj}c_{jj} + \sum_{k \neq j} b_{jk}^2 + \sum_{k \neq j} c_{kj}^2 + \sum_{k \neq j} c_{jk}^2 + \sum_{k \neq j} b_{kj}^2,$$

for  $j = 1, 2, \dots, n$ . Once again we consider  $\Delta_1$  only. Let the first row of  $Q^T$  be  $\mathbf{q} \equiv (q_1, \dots, q_n)$  and  $\mathbf{r}_1, \dots, \mathbf{r}_n$  be the rows of  $B$ . Then by a similar argument as for  $n = 3$ , we obtain the following analogue of (4):

$$\begin{aligned}
\Delta_1 &= \|B\|_F^2 - \sum_{k=2}^n \sum_{\ell=2}^n b_{k\ell}^2 - 2 \left[ \mathbf{q} \cdot (\mathbf{r}_1 \cdot \mathbf{q}^T, \dots, \mathbf{r}_n \cdot \mathbf{q}^T)^T \right] b_{11} \\
&\quad + \sum_{i=1}^n q_i^2 \|\mathbf{r}_i\|_2^2 + 2 \sum_{i=1}^n \sum_{k>i} q_i q_k \mathbf{r}_i \cdot \mathbf{r}_k^T + \sum_{i=1}^n \sum_{k>i} I_{ik},
\end{aligned} \tag{6}$$

where

$$I_{ik} \equiv \left| \begin{array}{cc} q_i & q_k \\ \mathbf{r}_i \cdot \mathbf{q}^T & \mathbf{r}_k \cdot \mathbf{q}^T \end{array} \right|^2.$$

Moreover, we have for  $k > 1$ ,

$$\begin{aligned} & 2q_1q_k\mathbf{r}_1 \cdot \mathbf{r}_k^T + I_{1k} \\ &= 2q_1q_k\mathbf{r}_1 \cdot \mathbf{r}_k^T + \left[ \sum_{j=1}^n q_j(q_1b_{kj} - q_kb_{1j}) \right]^2 \\ &\leq 2q_1q_k\mathbf{r}_1 \cdot \mathbf{r}_k^T + \|\mathbf{q}\|_2^2 \left[ \sum_{j=1}^n (q_1b_{kj} - q_kb_{1j})^2 \right] - \sum_{\ell=2}^n \left| \begin{matrix} q_1 & & q_\ell \\ q_1b_{k1} - q_kb_{11} & & q_1b_{k\ell} - q_kb_{1\ell} \end{matrix} \right|^2 \\ &= q_1^2\|\mathbf{r}_k\|_2^2 + q_k^2\|\mathbf{r}_1\|_2^2 - \sum_{\ell=2}^n J_{1k,\ell} \end{aligned}$$

with

$$J_{1k,\ell} \equiv \left| \begin{matrix} q_1 & & q_\ell \\ q_1b_{k1} - q_kb_{11} & & q_1b_{k\ell} - q_kb_{1\ell} \end{matrix} \right|^2.$$

For  $i \neq 1, k > i$ , we have

$$2q_iq_k\mathbf{r}_i \cdot \mathbf{r}_k^T + I_{ik} \leq q_i^2\|\mathbf{r}_k\|_2^2 + q_k^2\|\mathbf{r}_i\|_2^2.$$

Note that

$$\sum_{i=1}^n q_i^2\|\mathbf{r}_i\|_2^2 + \sum_{i=1}^n \sum_{k>i} (q_i^2\|\mathbf{r}_k\|_2^2 + q_k^2\|\mathbf{r}_i\|_2^2) = \sum_{i=1}^n q_i^2\|\mathbf{r}_i\|_2^2 + \sum_{i=1}^n \sum_{k \neq i} q_i^2\|\mathbf{r}_k\|_2^2 = \|B\|_F^2.$$

Putting all of these into (6), we obtain the following inequality which is similar to (5),

$$\begin{aligned} \Delta_1 &\leq 2\|B\|_F^2 - \sum_{k=2}^n \sum_{\ell=2}^n b_{k\ell}^2 - 2\left[ \mathbf{q} \cdot (\mathbf{r}_1 \cdot \mathbf{q}^T, \dots, \mathbf{r}_n \cdot \mathbf{q}^T)^T \right] b_{11} - \sum_{k=2}^n \sum_{\ell=2}^n J_{1k,\ell} \\ &= 2\|B\|_F^2 - \sum_{k=2}^n \sum_{\ell=2}^n b_{k\ell}^2 - 2q_1^2b_{11}^2 - 2\left( \sum_{k=2}^n \sum_{\ell=2}^n q_kq_\ell b_{k\ell} \right) b_{11} \\ &\quad - 2\left[ \sum_{k=2}^n q_1q_k(b_{1k} + b_{k1}) \right] b_{11} - \sum_{k=2}^n \sum_{\ell=2}^n J_{1k,\ell}. \end{aligned} \tag{7}$$

To dominate  $-2\left[ \sum_{k=2}^n q_1q_k(b_{1k} + b_{k1}) \right] b_{11}$  in (7), once again we note that  $\Delta_1 \leq 2\|B\|_F^2$  obviously holds when  $q_1^2 = 1$  (i.e.,  $q_2 = \dots = q_n = 0$ ). Therefore, we assume that  $q_1^2 \neq 1$  and denote  $M^2 \equiv q_2^2 + \dots + q_n^2 > 0$ . Thus, we have for  $k, \ell \geq 2$ ,

$$\begin{aligned} & -J_{1k,\ell} - 2q_kq_\ell \frac{q_1}{M^2} (q_\ell b_{k1} + q_k b_{1\ell}) b_{11} \\ &= -q_k^2q_\ell^2b_{11}^2 - (q_1q_\ell b_{k1} + q_1q_k b_{1\ell} - q_1^2b_{k\ell})^2 + 2q_kq_\ell b_{11} (q_1q_\ell b_{k1} + q_1q_k b_{1\ell} - q_1^2b_{k\ell}) \\ &\quad - 2q_kq_\ell \frac{q_1}{M^2} (q_\ell b_{k1} + q_k b_{1\ell}) b_{11} + 2q_kq_\ell \frac{q_1^2}{M^2} b_{11} b_{k\ell} - 2q_kq_\ell \frac{q_1^2}{M^2} b_{11} b_{k\ell} \\ &= -\left[ q_1q_\ell b_{k1} + q_1q_k b_{1\ell} - q_1^2b_{k\ell} - \frac{(M^2-1)}{M^2} q_kq_\ell b_{11} \right]^2 + \frac{q_1^4}{M^2} q_k^2q_\ell^2b_{11}^2 - q_k^2q_\ell^2b_{11}^2 \\ &\quad - 2q_kq_\ell \frac{q_1^2}{M^2} b_{11} b_{k\ell}, \end{aligned}$$

and

$$2 \sum_{k=2}^n \sum_{\ell=2}^n q_k q_\ell \frac{q_1}{M^2} (q_\ell b_{k1} + q_k b_{1\ell}) b_{11} = 2 \left[ \sum_{k=2}^n q_1 q_k (b_{1k} + b_{k1}) \right] b_{11}.$$

We remark that the above choice is inspired by the case when  $\ell = k$ . In such case, a  $q_k^2/M^2$  proportion of  $2q_1 q_k (b_{1k} + b_{k1}) b_{11}$  is grouped into  $J_{1k,k}$ . Although it is intuitive, it seems not straightforward to introduce a term in the denominator. We finally arrive at

$$\begin{aligned} \Delta_1 &\leq 2\|B\|_F^2 - \sum_{k=2}^n \sum_{\ell=2}^n b_{k\ell}^2 - 2q_1^2 b_{11}^2 - 2 \left( \sum_{k=2}^n \sum_{\ell=2}^n q_k q_\ell b_{k\ell} \right) b_{11} \\ &\quad + \sum_{k=2}^n \sum_{\ell=2}^n \left( \frac{q_1^4}{M^4} q_k^2 q_\ell^2 b_{11}^2 - q_k^2 q_\ell^2 b_{11}^2 - 2q_k q_\ell \frac{q_1^2}{M^2} b_{11} b_{k\ell} \right) \\ &= 2\|B\|_F^2 - \sum_{k=2}^n \sum_{\ell=2}^n b_{k\ell}^2 + \left[ \left( \frac{q_1^4}{M^4} - 1 \right) \left( \sum_{k=2}^n q_k^2 \right) \left( \sum_{\ell=2}^n q_\ell^2 \right) - 2q_1^2 \right] b_{11}^2 \\ &\quad - 2 \sum_{k=2}^n \sum_{\ell=2}^n q_k q_\ell \left( 1 + \frac{q_1^2}{M^2} \right) b_{11} b_{k\ell} \\ &= 2\|B\|_F^2 - \sum_{k=2}^n \sum_{\ell=2}^n b_{k\ell}^2 + \left[ (1 - M^2)^2 - M^4 - 2(1 - M^2) \right] b_{11}^2 \\ &\quad - \frac{2}{M^2} \sum_{k=2}^n \sum_{\ell=2}^n q_k q_\ell b_{11} b_{k\ell} \\ &\leq 2\|B\|_F^2 - b_{11}^2 + \frac{1}{M^4} \left( \sum_{k=2}^n \sum_{\ell=2}^n q_k^2 q_\ell^2 \right) b_{11}^2 = 2\|B\|_F^2. \end{aligned}$$

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