

On the accuracy of ancestral sequence reconstruction for ultrametric trees with parsimony

Supplementary material

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1 Proof of Lemma 1

To prove Lemma 1 we show that for any rooted binary phylogenetic tree T under a symmetric 4-state substitution model

$$P_\alpha(X) \geq P_\beta(X), \quad (1.1)$$

$$P_{\alpha\beta}(X) \geq P_{\beta\gamma}(X), \quad (1.2)$$

$$P_{\alpha\beta\gamma}(X) \geq P_{\beta\gamma\delta}(X) \quad (1.3)$$

by induction on n . For $n = 2$ the subtrees Y_1 and Y_2 both contain one leaf, which leads to

$$\begin{aligned} P_\alpha(X) &= (1 - 3p_1)(1 - 3p_2), \\ P_\beta(X) &= p_1p_2, \\ P_{\alpha\beta}(X) &= (1 - 3p_1)p_2 + p_1(1 - 3p_2), \\ P_{\beta\gamma}(X) &= 2p_1p_2, \\ P_{\alpha\beta\gamma}(X) &= 0, \\ P_{\beta\gamma\delta}(X) &= 0. \end{aligned}$$

Therefore

$$\begin{aligned} P_\alpha(X) - P_\beta(X) &= (1 - 3p_1)(1 - 3p_2) - p_1p_2 = 1 - 3p_1 - 3p_2 + 9p_1p_2 - p_1p_2 = 1 - 3p_1 - 3p_2 + 8p_1p_2 \\ &= \underbrace{(1 - 4p_1)}_{\geq 0} \underbrace{(1 - 4p_2)}_{\geq 0} + p_1 \underbrace{(1 - 4p_2)}_{\geq 0} + \underbrace{(1 - 4p_1)}_{\geq 0} p_2 \geq 0 \text{ as } 0 \leq p_1, p_2 \leq \frac{1}{4}. \end{aligned}$$

Moreover

$$P_{\alpha\beta}(X) - P_{\beta\gamma}(X) = (1 - 3p_1)p_2 + p_1(1 - 3p_2) - 2p_1p_2 = p_1 \underbrace{(1 - 4p_2)}_{\geq 0} + \underbrace{(1 - 4p_1)}_{\geq 0} p_2 \geq 0 \text{ as } 0 \leq p_1, p_2 \leq \frac{1}{4},$$

and

$$P_{\alpha\beta\gamma}(X) - P_{\beta\gamma\delta}(X) = 0 - 0 = 0 \geq 0,$$

which completes the base case of the induction. For the inductive step we first state some more recursions using (9), (10), (11), (12) and (13):

$$\begin{aligned} P_\beta(X) &= P_{(\beta)}(Y_1)P_{(\beta)}(Y_2) + P_{(\beta)}(Y_1)P_{(\alpha\beta)}(Y_2) + P_{(\alpha\beta)}(Y_1)P_{(\beta)}(Y_2) \\ &\quad + 2P_{(\beta)}(Y_1)P_{(\beta\gamma)}(Y_2) + 2P_{(\beta\gamma)}(Y_1)P_{(\beta)}(Y_2) + 2P_{(\alpha\beta)}(Y_1)P_{(\beta\gamma)}(Y_2) \\ &\quad + 2P_{(\beta\gamma)}(Y_1)P_{(\alpha\beta)}(Y_2) + 2P_{(\beta\gamma)}(Y_1)P_{(\beta\gamma)}(Y_2) + 2P_{(\beta)}(Y_1)P_{(\alpha\beta\gamma)}(Y_2) \\ &\quad + 2P_{(\alpha\beta\gamma)}(Y_1)P_{(\beta)}(Y_2) + P_{(\beta)}(Y_1)P_{(\beta\gamma\delta)}(Y_2) + P_{(\beta\gamma\delta)}(Y_1)P_{(\beta)}(Y_2) \\ &\quad + 2P_{(\beta\gamma)}(Y_1)P_{(\alpha\beta\gamma)}(Y_2) + 2P_{(\alpha\beta\gamma)}(Y_1)P_{(\beta\gamma)}(Y_2) + P_{(\alpha\beta)}(Y_1)P_{(\beta\gamma\delta)}(Y_2) \\ &\quad + P_{(\beta\gamma\delta)}(Y_1)P_{(\alpha\beta)}(Y_2) + P_{(\beta)}(Y_1)P_{(\alpha\beta\gamma\delta)}(Y_2) + P_{(\alpha\beta\gamma\delta)}(Y_1)P_{(\beta)}(Y_2), \end{aligned} \quad (1.4)$$

$$\begin{aligned}
P_{\beta\gamma}(X) &= P_{(\beta)}(Y_1)P_{(\gamma)}(Y_2) + P_{(\gamma)}(Y_1)P_{(\beta)}(Y_2) + P_{(\beta\gamma)}(Y_1)P_{(\beta\gamma)}(Y_2) \\
&\quad + P_{(\beta\gamma)}(Y_1)P_{(\alpha\beta\gamma)}(Y_2) + P_{(\alpha\beta\gamma)}(Y_1)P_{(\beta\gamma)}(Y_2) + P_{(\beta\gamma)}(Y_1)P_{(\beta\gamma\delta)}(Y_2) \\
&\quad + P_{(\beta\gamma\delta)}(Y_1)P_{(\beta\gamma)}(Y_2) + P_{(\alpha\beta\gamma)}(Y_1)P_{(\beta\gamma\delta)}(Y_2) + P_{(\beta\gamma\delta)}(Y_1)P_{(\alpha\beta\gamma)}(Y_2) \\
&\quad + P_{(\beta\gamma)}(Y_1)P_{(\alpha\beta\gamma\delta)}(Y_2) + P_{(\alpha\beta\gamma\delta)}(Y_1)P_{(\beta\gamma)}(Y_2),
\end{aligned} \tag{1.5}$$

$$\begin{aligned}
P_{\beta\gamma\delta}(X) &= 3P_{(\beta)}(Y_1)P_{(\beta\gamma)}(Y_2) + 3P_{(\beta\gamma)}(Y_1)P_{(\beta)}(Y_2) + P_{(\beta\gamma\delta)}(Y_1)P_{(\beta\gamma\delta)}(Y_2) \\
&\quad + P_{(\beta\gamma\delta)}(Y_1)P_{(\alpha\beta\gamma\delta)}(Y_2) + P_{(\alpha\beta\gamma\delta)}(Y_1)P_{(\beta\gamma\delta)}(Y_2).
\end{aligned} \tag{1.6}$$

Furthermore, for $i \in \{1, 2\}$ we define $P_i := 1 - 4p_i$, and similarly $P := 1 - 4p$. Moreover, we have that for $i \in \{1, 2\}$

$$\begin{aligned}
P_{(\alpha)}(Y_i) - P_{(\beta)}(Y_i) &= (1 - 3p_i)P_{\alpha}(Y_i) + 3p_iP_{\beta}(Y_i) - (1 - p_i)P_{\beta}(Y_i) - p_iP_{\alpha}(Y_i) \\
&\quad \text{by (8), (9)} \\
&= (1 - 4p_i)P_{\alpha}(Y_i) - (1 - 4p_i)P_{\beta}(Y_i) \\
&= P_i \left(P_{\alpha}(Y_i) - P_{\beta}(Y_i) \right) \\
&\quad \text{by the definition of } P_i
\end{aligned} \tag{1.7}$$

and thus

$$P_{(\alpha)}(Y_i) = P_{(\beta)}(Y_i) + P_i \left(P_{\alpha}(Y_i) - P_{\beta}(Y_i) \right). \tag{1.8}$$

In the same manner by (10), (11), (12) and (13) we can see that

$$P_{(\alpha\beta)}(Y_i) - P_{(\beta\gamma)}(Y_i) = P_i \left(P_{\alpha\beta}(Y_i) - P_{\beta\gamma}(Y_i) \right), \tag{1.9}$$

$$P_{(\alpha\beta\gamma)}(Y_i) - P_{(\beta\gamma\delta)}(Y_i) = P_i \left(P_{\alpha\beta\gamma}(Y_i) - P_{\beta\gamma\delta}(Y_i) \right). \tag{1.10}$$

Therefore

$$P_{(\alpha\beta)}(Y_i) = P_{(\beta\gamma)}(Y_i) + P_i \left(P_{\alpha\beta}(Y_i) - P_{\beta\gamma}(Y_i) \right), \tag{1.11}$$

$$P_{(\alpha\beta\gamma)}(Y_i) = P_{(\beta\gamma\delta)}(Y_i) + P_i \left(P_{\alpha\beta\gamma}(Y_i) - P_{\beta\gamma\delta}(Y_i) \right). \tag{1.12}$$

Additionally we have the following: choose sets A_1, A_2 from $\{\{\alpha\}, \{\alpha\beta\}, \{\alpha\beta\gamma\}\}$ and B_1, B_2 from $\{\{\beta\}, \{\beta\gamma\}, \{\beta\gamma\delta\}\}$ such that for $i \in \{1, 2\}$ $|A_i| = |B_i|$, respectively. Then we have that

$$\begin{aligned}
&P_{(A_1)}(Y_1)P_{(A_2)}(Y_2) - P_{(B_1)}(Y_1)P_{(B_2)}(Y_2) \\
&= \left(P_{(B_1)}(Y_1) + P_1 \left(P_{A_1}(Y_1) - P_{B_1}(Y_1) \right) \right) \left(P_{(B_2)}(Y_2) + P_2 \left(P_{A_2}(Y_2) - P_{B_2}(Y_2) \right) \right) \\
&\quad - P_{(B_1)}(Y_1)P_{(B_2)}(Y_2) \\
&\quad \text{by (1.8), (1.11) or (1.12)} \\
&= P_{(B_1)}(Y_1)P_{(B_2)}(Y_2) + P_{(B_1)}(Y_1)P_2 \left(P_{A_2}(Y_2) - P_{B_2}(Y_2) \right) \\
&\quad + P_{(B_2)}(Y_2)P_1 \left(P_{A_1}(Y_1) - P_{B_1}(Y_1) \right) \\
&\quad + P_1P_2 \left(P_{A_1}(Y_1) - P_{B_1}(Y_1) \right) \left(P_{A_2}(Y_2) - P_{B_2}(Y_2) \right) - P_{(B_1)}(Y_1)P_{(B_2)}(Y_2) \\
&= P_{(B_1)}(Y_1)P_2 \left(P_{A_2}(Y_2) - P_{B_2}(Y_2) \right) + P_{(B_2)}(Y_2)P_1 \left(P_{A_1}(Y_1) - P_{B_1}(Y_1) \right) \\
&\quad + P_1P_2 \left(P_{A_1}(Y_1) - P_{B_1}(Y_1) \right) \left(P_{A_2}(Y_2) - P_{B_2}(Y_2) \right).
\end{aligned} \tag{1.13}$$

Now suppose that T has n taxa and that (1.1),(1.2) and (1.3) are true for all trees having fewer than n taxa. Note that therefore (1.13) is non-negative, since Y_1 and Y_2 contain both fewer than n taxa. Then

$$\begin{aligned}
& P_\alpha(X) - P_\beta(X) \\
&= P_{(\alpha)}(Y_1)P_{(\alpha)}(Y_2) + 3P_{(\alpha)}(Y_1)P_{(\alpha\beta)}(Y_2) + 3P_{(\alpha\beta)}(Y_1)P_{(\alpha)}(Y_2) \\
&\quad + 3P_{(\alpha)}(Y_1)P_{(\alpha\beta\gamma)}(Y_2) + 3P_{(\alpha\beta\gamma)}(Y_1)P_{(\alpha)}(Y_2) + 6P_{(\alpha\beta)}(Y_1)P_{(\alpha\beta)}(Y_2) \\
&\quad + 3P_{(\alpha\beta)}(Y_1)P_{(\alpha\beta\gamma)}(Y_2) + 3P_{(\alpha\beta\gamma)}(Y_1)P_{(\alpha\beta)}(Y_2) + P_{(\alpha)}(Y_1)P_{(\alpha\beta\gamma\delta)}(Y_2) \\
&\quad + P_{(\alpha\beta\gamma\delta)}(Y_1)P_{(\alpha)}(Y_2) - P_{(\beta)}(Y_1)P_{(\beta)}(Y_2) - P_{(\beta)}(Y_1)P_{(\alpha\beta)}(Y_2) \\
&\quad - P_{(\alpha\beta)}(Y_1)P_{(\beta)}(Y_2) - 2P_{(\beta)}(Y_1)P_{(\beta\gamma)}(Y_2) - 2P_{(\beta\gamma)}(Y_1)P_{(\beta)}(Y_2) \\
&\quad - 2P_{(\alpha\beta)}(Y_1)P_{(\beta\gamma)}(Y_2) - 2P_{(\beta\gamma)}(Y_1)P_{(\alpha\beta)}(Y_2) - 2P_{(\beta\gamma)}(Y_1)P_{(\beta\gamma)}(Y_2) \\
&\quad - 2P_{(\beta)}(Y_1)P_{(\alpha\beta\gamma)}(Y_2) - 2P_{(\alpha\beta\gamma)}(Y_1)P_{(\beta)}(Y_2) - P_{(\beta)}(Y_1)P_{(\beta\gamma\delta)}(Y_2) \\
&\quad - P_{(\beta\gamma\delta)}(Y_1)P_{(\beta)}(Y_2) - 2P_{(\beta\gamma)}(Y_1)P_{(\alpha\beta\gamma)}(Y_2) - 2P_{(\alpha\beta\gamma)}(Y_1)P_{(\beta\gamma)}(Y_2) \\
&\quad - P_{(\alpha\beta)}(Y_1)P_{(\beta\gamma\delta)}(Y_2) - P_{(\beta\gamma\delta)}(Y_1)P_{(\alpha\beta)}(Y_2) - P_{(\beta)}(Y_1)P_{(\alpha\beta\gamma\delta)}(Y_2) \\
&\quad - P_{(\alpha\beta\gamma\delta)}(Y_1)P_{(\beta)}(Y_2) \\
&\text{by (15) and (1.4)} \\
&= P_{(\alpha)}(Y_1)P_{(\alpha)}(Y_2) - P_{(\beta)}(Y_1)P_{(\beta)}(Y_2) \\
&\quad + 2P_{(\alpha\beta)}(Y_1)P_{(\alpha\beta)}(Y_2) - 2P_{(\beta\gamma)}(Y_1)P_{(\beta\gamma)}(Y_2) \\
&\quad + P_{(\alpha\beta)}(Y_2)\left(P_{(\alpha)}(Y_1) - P_{(\beta)}(Y_1)\right) + P_{(\alpha\beta)}(Y_1)\left(P_{(\alpha)}(Y_2) - P_{(\beta)}(Y_2)\right) \\
&\quad + 2P_{(\alpha)}(Y_1)P_{(\alpha\beta)}(Y_2) - 2P_{(\beta)}(Y_1)P_{(\beta\gamma)}(Y_2) \\
&\quad + 2P_{(\alpha\beta)}(Y_1)P_{(\alpha)}(Y_2) - 2P_{(\beta\gamma)}(Y_1)P_{(\beta)}(Y_2) \\
&\quad + 2P_{(\alpha\beta\gamma)}(Y_2)\left(P_{(\alpha)}(Y_1) - P_{(\beta)}(Y_1)\right) + 2P_{(\alpha\beta\gamma)}(Y_1)\left(P_{(\alpha)}(Y_2) - P_{(\beta)}(Y_2)\right) \\
&\quad + P_{(\alpha)}(Y_1)P_{(\alpha\beta\gamma)}(Y_2) - P_{(\beta)}(Y_1)P_{(\beta\gamma\delta)}(Y_2) \\
&\quad + P_{(\alpha\beta\gamma)}(Y_1)P_{(\alpha)}(Y_2) - P_{(\beta\gamma\delta)}(Y_1)P_{(\beta)}(Y_2) \\
&\quad + 2P_{(\alpha\beta)}(Y_2)\left(P_{(\alpha\beta)}(Y_1) - P_{(\beta\gamma)}(Y_1)\right) + 2P_{(\alpha\beta)}(Y_1)\left(P_{(\alpha\beta)}(Y_2) - P_{(\beta\gamma)}(Y_2)\right) \\
&\quad + 2P_{(\alpha\beta\gamma)}(Y_2)\left(P_{(\alpha\beta)}(Y_1) - P_{(\beta\gamma)}(Y_1)\right) + 2P_{(\alpha\beta\gamma)}(Y_1)\left(P_{(\alpha\beta)}(Y_2) - P_{(\beta\gamma)}(Y_2)\right) \\
&\quad + P_{(\alpha\beta)}(Y_2)\left(P_{(\alpha\beta\gamma)}(Y_1) - P_{(\beta\gamma\delta)}(Y_1)\right) + P_{(\alpha\beta)}(Y_1)\left(P_{(\alpha\beta\gamma)}(Y_2) - P_{(\beta\gamma\delta)}(Y_2)\right) \\
&\quad + P_{(\alpha\beta\gamma\delta)}(Y_2)\left(P_{(\alpha)}(Y_1) - P_{(\beta)}(Y_1)\right) + P_{(\alpha\beta\gamma\delta)}(Y_1)\left(P_{(\alpha)}(Y_2) - P_{(\beta)}(Y_2)\right) \\
&= P_{(\alpha)}(Y_1)P_{(\alpha)}(Y_2) - P_{(\beta)}(Y_1)P_{(\beta)}(Y_2) \\
&\quad + 2\left(P_{(\alpha\beta)}(Y_1)P_{(\alpha\beta)}(Y_2) - P_{(\beta\gamma)}(Y_1)P_{(\beta\gamma)}(Y_2)\right) \\
&\quad + 2\left(P_{(\alpha)}(Y_1)P_{(\alpha\beta)}(Y_2) - P_{(\beta)}(Y_1)P_{(\beta\gamma)}(Y_2)\right) \\
&\quad + 2\left(P_{(\alpha\beta)}(Y_1)P_{(\alpha)}(Y_2) - 2P_{(\beta\gamma)}(Y_1)P_{(\beta)}(Y_2)\right) \\
&\quad + P_{(\alpha)}(Y_1)P_{(\alpha\beta\gamma)}(Y_2) - P_{(\beta)}(Y_1)P_{(\beta\gamma\delta)}(Y_2) \\
&\quad + P_{(\alpha\beta\gamma)}(Y_1)P_{(\alpha)}(Y_2) - P_{(\beta\gamma\delta)}(Y_1)P_{(\beta)}(Y_2) \\
&\quad + \left(P_{(\alpha)}(Y_1) - P_{(\beta)}(Y_1)\right)\left(P_{(\alpha\beta)}(Y_2) + 2P_{(\alpha\beta\gamma)}(Y_2) + P_{(\alpha\beta\gamma\delta)}(Y_2)\right) \\
&\quad + \left(P_{(\alpha)}(Y_2) - P_{(\beta)}(Y_2)\right)\left(P_{(\alpha\beta)}(Y_1) + 2P_{(\alpha\beta\gamma)}(Y_1) + P_{(\alpha\beta\gamma\delta)}(Y_1)\right) \\
&\quad + \left(P_{(\alpha\beta)}(Y_1) - P_{(\beta\gamma)}(Y_1)\right)\left(2P_{(\alpha\beta)}(Y_2) + 2P_{(\alpha\beta\gamma)}(Y_2)\right) \\
&\quad + \left(P_{(\alpha\beta)}(Y_2) - P_{(\beta\gamma)}(Y_2)\right)\left(2P_{(\alpha\beta)}(Y_1) + 2P_{(\alpha\beta\gamma)}(Y_1)\right) \\
&\quad + \left(P_{(\alpha\beta\gamma)}(Y_1) - P_{(\beta\gamma\delta)}(Y_1)\right)P_{(\alpha\beta)}(Y_2) + \left(P_{(\alpha\beta\gamma)}(Y_2) - P_{(\beta\gamma\delta)}(Y_2)\right)P_{(\alpha\beta)}(Y_1)
\end{aligned}$$

$$\begin{aligned}
&= P_{(\alpha)}(Y_1)P_{(\alpha)}(Y_2) - P_{(\beta)}(Y_1)P_{(\beta)}(Y_2) \\
&\quad + 2\left(P_{(\alpha\beta)}(Y_1)P_{(\alpha\beta)}(Y_2) - P_{(\beta\gamma)}(Y_1)P_{(\beta\gamma)}(Y_2)\right) \\
&\quad + 2\left(P_{(\alpha)}(Y_1)P_{(\alpha\beta)}(Y_2) - P_{(\beta)}(Y_1)P_{(\beta\gamma)}(Y_2)\right) \\
&\quad + 2\left(P_{(\alpha\beta)}(Y_1)P_{(\alpha)}(Y_2) - P_{(\beta\gamma)}(Y_1)P_{(\beta)}(Y_2)\right) \\
&\quad + P_{(\alpha)}(Y_1)P_{(\alpha\beta\gamma)}(Y_2) - P_{(\beta)}(Y_1)P_{(\beta\gamma\delta)}(Y_2) \\
&\quad + P_{(\alpha\beta\gamma)}(Y_1)P_{(\alpha)}(Y_2) - P_{(\beta\gamma\delta)}(Y_1)P_{(\beta)}(Y_2) \\
&\quad + P_1\left(P_{\alpha}(Y_1) - P_{\beta}(Y_1)\right)\left(P_{(\alpha\beta)}(Y_2) + 2P_{(\alpha\beta\gamma)}(Y_2) + P_{(\alpha\beta\gamma\delta)}(Y_2)\right) \\
&\quad + P_2\left(P_{\alpha}(Y_2) - P_{\beta}(Y_2)\right)\left(P_{(\alpha\beta)}(Y_1) + 2P_{(\alpha\beta\gamma)}(Y_1) + P_{(\alpha\beta\gamma\delta)}(Y_1)\right) \\
&\quad + P_1\left(P_{\alpha\beta}(Y_1) - P_{\beta\gamma}(Y_1)\right)\left(2P_{(\alpha\beta)}(Y_2) + 2P_{(\alpha\beta\gamma)}(Y_2)\right) \\
&\quad + P_2\left(P_{\alpha\beta}(Y_2) - P_{\beta\gamma}(Y_2)\right)\left(2P_{(\alpha\beta)}(Y_1) + 2P_{(\alpha\beta\gamma)}(Y_1)\right) \\
&\quad + P_1\left(P_{\alpha\beta\gamma}(Y_1) - P_{\beta\gamma\delta}(Y_1)\right)P_{(\alpha\beta)}(Y_2) + P_2\left(P_{\alpha\beta\delta}(Y_2) - P_{\beta\gamma\delta}(Y_2)\right)P_{(\alpha\beta)}(Y_1) \\
&\text{by (1.7), (1.9) and (1.10).}
\end{aligned}$$

By (1.13) and the inductive assumption this term is non-negative, and therefore concludes the proof for $P_{\alpha}(X) \geq P_{\beta}(X)$. We now proceed with the second part of Lemma 1.

$$\begin{aligned}
&P_{\alpha\beta}(X) - P_{\beta\gamma}(X) \\
&= P_{(\alpha)}(Y_1)P_{(\beta)}(Y_2) + P_{(\beta)}(Y_1)P_{(\alpha)}(Y_2) + P_{(\alpha\beta)}(Y_1)P_{(\alpha\beta)}(Y_2) \\
&\quad + 2P_{(\alpha\beta)}(Y_1)P_{(\alpha\beta\gamma)}(Y_2) + 2P_{(\alpha\beta\gamma)}(Y_1)P_{(\alpha\beta)}(Y_2) + P_{(\alpha\beta)}(Y_1)P_{(\alpha\beta\gamma\delta)}(Y_2) \\
&\quad + P_{(\alpha\beta\gamma\delta)}(Y_1)P_{(\alpha\beta)}(Y_2) + 2P_{(\alpha\beta\gamma)}(Y_1)P_{(\alpha\beta\gamma)}(Y_2) - 2P_{(\beta)}(Y_1)P_{(\beta)}(Y_2) \\
&\quad - P_{(\beta\gamma)}(Y_1)P_{(\beta\gamma)}(Y_2) - P_{(\beta\gamma)}(Y_1)P_{(\alpha\beta\gamma)}(Y_2) - P_{(\alpha\beta\gamma)}(Y_1)P_{(\beta\gamma)}(Y_2) \\
&\quad - P_{(\beta\gamma)}(Y_1)P_{(\beta\gamma\delta)}(Y_2) - P_{(\beta\gamma\delta)}(Y_1)P_{(\beta\gamma)}(Y_2) - P_{(\alpha\beta\gamma)}(Y_1)P_{(\beta\gamma\delta)}(Y_2) \\
&\quad - P_{(\beta\gamma\delta)}(Y_1)P_{(\alpha\beta\gamma)}(Y_2) - P_{(\beta\gamma)}(Y_1)P_{(\alpha\beta\gamma\delta)}(Y_2) - P_{(\alpha\beta\gamma\delta)}(Y_1)P_{(\beta\gamma)}(Y_2) \\
&\text{by (9), (16) and (1.5)} \\
&= P_{(\beta)}(Y_2)\left(P_{(\alpha)}(Y_1) - P_{(\beta)}(Y_1)\right) + P_{(\beta)}(Y_1)\left(P_{(\alpha)}(Y_2) - P_{(\beta)}(Y_2)\right) \\
&\quad + P_{(\alpha\beta)}(Y_1)P_{(\alpha\beta)}(Y_2) - P_{(\beta\gamma)}(Y_1)P_{(\beta\gamma)}(Y_2) \\
&\quad + P_{(\alpha\beta\gamma)}(Y_2)\left(P_{(\alpha\beta)}(Y_1) - P_{(\beta\gamma)}(Y_1)\right) \\
&\quad + P_{(\alpha\beta\gamma)}(Y_1)\left(P_{(\alpha\beta)}(Y_2) - P_{(\beta\gamma)}(Y_2)\right) \\
&\quad + P_{(\alpha\beta)}(Y_1)P_{(\alpha\beta\gamma)}(Y_2) - P_{(\beta\gamma)}(Y_1)P_{(\beta\gamma\delta)}(Y_2) \\
&\quad + P_{(\alpha\beta\gamma)}(Y_1)P_{(\alpha\beta)}(Y_2) - P_{(\beta\gamma\delta)}(Y_1)P_{(\beta\gamma)}(Y_2) \\
&\quad + P_{(\alpha\beta\gamma)}(Y_2)\left(P_{(\alpha\beta\gamma)}(Y_1) - P_{(\beta\gamma\delta)}(Y_1)\right) \\
&\quad + P_{(\alpha\beta\gamma)}(Y_1)\left(P_{(\alpha\beta\gamma)}(Y_2) - P_{(\beta\gamma\delta)}(Y_2)\right) \\
&\quad + P_{(\alpha\beta\gamma\delta)}(Y_2)\left(P_{(\alpha\beta)}(Y_1) - P_{(\beta\gamma)}(Y_1)\right) \\
&\quad + P_{(\alpha\beta\gamma\delta)}(Y_1)\left(P_{(\alpha\beta)}(Y_2) - P_{(\beta\gamma)}(Y_2)\right)
\end{aligned}$$

$$\begin{aligned}
&= P_{(\alpha\beta)}(Y_1)P_{(\alpha\beta)}(Y_2) - P_{(\beta\gamma)}(Y_1)P_{(\beta\gamma)}(Y_2) \\
&\quad + P_{(\alpha\beta)}(Y_1)P_{(\alpha\beta\gamma)}(Y_2) - P_{(\beta\gamma)}(Y_1)P_{(\beta\gamma\delta)}(Y_2) \\
&\quad + P_{(\alpha\beta\gamma)}(Y_1)P_{(\alpha\beta)}(Y_2) - P_{(\beta\gamma\delta)}(Y_1)P_{(\beta\gamma)}(Y_2) \\
&\quad + P_{(\beta)}(Y_2)\left(P_{(\alpha)}(Y_1) - P_{(\beta)}(Y_1)\right) + P_{(\beta)}(Y_1)\left(P_{(\alpha)}(Y_2) - P_{(\beta)}(Y_2)\right) \\
&\quad + \left(P_{(\alpha\beta\gamma)}(Y_2) + P_{(\alpha\beta\gamma\delta)}(Y_2)\right)\left(P_{(\alpha\beta)}(Y_1) - P_{(\beta\gamma)}(Y_1)\right) \\
&\quad + \left(P_{(\alpha\beta\gamma)}(Y_1) + P_{(\alpha\beta\gamma\delta)}(Y_1)\right)\left(P_{(\alpha\beta)}(Y_2) - P_{(\beta\gamma)}(Y_2)\right) \\
&\quad + P_{(\alpha\beta\gamma)}(Y_2)\left(P_{(\alpha\beta\gamma)}(Y_1) - P_{(\beta\gamma\delta)}(Y_1)\right) \\
&\quad + P_{(\alpha\beta\gamma)}(Y_1)\left(P_{(\alpha\beta\gamma)}(Y_2) - P_{(\beta\gamma\delta)}(Y_2)\right) \\
&= P_{(\alpha\beta)}(Y_1)P_{(\alpha\beta)}(Y_2) - P_{(\beta\gamma)}(Y_1)P_{(\beta\gamma)}(Y_2) \\
&\quad + P_{(\alpha\beta)}(Y_1)P_{(\alpha\beta\gamma)}(Y_2) - P_{(\beta\gamma)}(Y_1)P_{(\beta\gamma\delta)}(Y_2) \\
&\quad + P_{(\alpha\beta\gamma)}(Y_1)P_{(\alpha\beta)}(Y_2) - P_{(\beta\gamma\delta)}(Y_1)P_{(\beta\gamma)}(Y_2) \\
&\quad + P_{(\beta)}(Y_2)P_1\left(P_{\alpha}(Y_1) - P_{\beta}(Y_1)\right) + P_{(\beta)}(Y_1)P_2\left(P_{\alpha}(Y_2) - P_{\beta}(Y_2)\right) \\
&\quad + \left(P_{(\alpha\beta\gamma)}(Y_2) + P_{(\alpha\beta\gamma\delta)}(Y_2)\right)P_1\left(P_{\alpha\beta}(Y_1) - P_{\beta\gamma}(Y_1)\right) \\
&\quad + \left(P_{(\alpha\beta\gamma)}(Y_1) + P_{(\alpha\beta\gamma\delta)}(Y_1)\right)P_2\left(P_{\alpha\beta}(Y_2) - P_{\beta\gamma}(Y_2)\right) \\
&\quad + P_{(\alpha\beta\gamma)}(Y_2)P_1\left(P_{\alpha\beta\gamma}(Y_1) - P_{\beta\gamma\delta}(Y_1)\right) \\
&\quad + P_{(\alpha\beta\gamma)}(Y_1)P_2\left(P_{\alpha\beta\gamma}(Y_2) - P_{\beta\gamma\delta}(Y_2)\right) \\
&\text{by (1.7), (1.9) and (1.10).}
\end{aligned}$$

Again by (1.13) and the inductive assumption this term is non-negative, and therefore concludes the proof for $P_{\alpha\beta}(X) \geq P_{\beta\gamma}(X)$. Moreover we have

$$\begin{aligned}
&P_{\alpha\beta\gamma}(X) - P_{\beta\gamma\delta}(X) \\
&= P_{(\alpha)}(Y_1)P_{(\beta\gamma)}(Y_2) + P_{(\beta\gamma)}(Y_1)P_{(\alpha)}(Y_2) + 2P_{(\beta)}(Y_1)P_{(\alpha\beta)}(Y_2) \\
&\quad + 2P_{(\alpha\beta)}(Y_1)P_{(\beta)}(Y_2) + P_{(\alpha\beta\gamma)}(Y_1)P_{(\alpha\beta\gamma)}(Y_2) + P_{(\alpha\beta\gamma)}(Y_1)P_{(\alpha\beta\gamma\delta)}(Y_2) \\
&\quad + P_{(\alpha\beta\gamma\delta)}(Y_1)P_{(\alpha\beta\gamma)}(Y_2) - 3P_{(\beta)}(Y_1)P_{(\beta\gamma)}(Y_2) - 3P_{(\beta\gamma)}(Y_1)P_{(\beta)}(Y_2) \\
&\quad - P_{(\beta\gamma\delta)}(Y_1)P_{(\beta\gamma\delta)}(Y_2) - P_{(\beta\gamma\delta)}(Y_1)P_{(\alpha\beta\gamma\delta)}(Y_2) - P_{(\alpha\beta\gamma\delta)}(Y_1)P_{(\beta\gamma\delta)}(Y_2) \\
&\text{by (1.7) and (1.6)} \\
&= P_{(\beta\gamma)}(Y_2)\left(P_{(\alpha)}(Y_1) - P_{(\beta)}(Y_1)\right) + P_{(\beta\gamma)}(Y_1)\left(P_{(\alpha)}(Y_2) - P_{(\beta)}(Y_2)\right) \\
&\quad + 2P_{(\beta)}(Y_2)\left(P_{(\alpha\beta)}(Y_1) - P_{(\beta\gamma)}(Y_1)\right) + 2P_{(\beta)}(Y_1)\left(P_{(\alpha\beta)}(Y_2) - P_{(\beta\gamma)}(Y_2)\right) \\
&\quad + P_{(\alpha\beta\gamma)}(Y_1)P_{(\alpha\beta\gamma)}(Y_2) - P_{(\beta\gamma\delta)}(Y_1)P_{(\beta\gamma\delta)}(Y_2) \\
&\quad + P_{(\alpha\beta\gamma\delta)}(Y_2)\left(P_{(\alpha\beta\gamma)}(Y_1) - P_{(\beta\gamma\delta)}(Y_1)\right) \\
&\quad + P_{(\alpha\beta\gamma\delta)}(Y_1)\left(P_{(\alpha\beta\gamma)}(Y_2) - P_{(\beta\gamma\delta)}(Y_2)\right) \\
&= P_{(\beta\gamma)}(Y_2)P_1\left(P_{\alpha}(Y_1) - P_{\beta}(Y_1)\right) + P_{(\beta\gamma)}(Y_1)P_2\left(P_{\alpha}(Y_2) - P_{\beta}(Y_2)\right) \\
&\quad + 2P_{(\beta)}(Y_2)P_1\left(P_{\alpha\beta}(Y_1) - P_{\beta\gamma}(Y_1)\right) + 2P_{(\beta)}(Y_1)P_2\left(P_{\alpha\beta}(Y_2) - P_{\beta\gamma}(Y_2)\right) \\
&\quad + P_{(\alpha\beta\gamma)}(Y_1)P_{(\alpha\beta\gamma)}(Y_2) - P_{(\beta\gamma\delta)}(Y_1)P_{(\beta\gamma\delta)}(Y_2) \\
&\quad + P_{(\alpha\beta\gamma\delta)}(Y_2)P_1\left(P_{\alpha\beta\gamma}(Y_1) - P_{\beta\gamma\delta}(Y_1)\right) \\
&\quad + P_{(\alpha\beta\gamma\delta)}(Y_1)P_2\left(P_{\alpha\beta\gamma}(Y_2) - P_{\beta\gamma\delta}(Y_2)\right) \\
&\text{by (1.7), (1.9) and (1.10).}
\end{aligned}$$

By (1.13) and the inductive assumption $P_{\alpha\beta\gamma}(X) - P_{\beta\gamma\delta}(X)$ is non-negative, and therefore concludes the proof of the last part of Lemma 1. \square

2 Extension to the proof of Theorem 1

First of all we state some equations for $i \in \{1, 2\}$ which helps to show (19).

$$\begin{aligned}
1 &= P_\alpha(Y_i) + P_\beta(Y_i) + P_\gamma(Y_i) + P_\delta(Y_i) + P_{\alpha\beta}(Y_i) + P_{\alpha\gamma}(Y_i) + P_{\alpha\delta}(Y_i) + P_{\beta\gamma}(Y_i) \\
&\quad + P_{\beta\delta}(Y_i) + P_{\gamma\delta}(Y_i) + P_{\alpha\beta\gamma}(Y_i) + P_{\alpha\beta\delta}(Y_i) + P_{\alpha\gamma\delta}(Y_i) + P_{\beta\gamma\delta}(Y_i) + P_{\alpha\beta\gamma\delta}(Y_i) \\
&= P_\alpha(Y_i) + 3P_\beta(Y_i) + 3P_{\alpha\beta}(Y_i) + 3P_{\beta\gamma}(Y_i) + 3P_{\alpha\beta\gamma}(Y_i) + P_{\beta\gamma\delta}(Y_i) + P_{\alpha\beta\gamma\delta}(Y_i) \\
&\text{by (7), (4), (5)}.
\end{aligned} \tag{2.1}$$

By (2.1) we have that

$$\begin{aligned}
&3P_\beta(Y_i) \\
&= 1 - P_\alpha(Y_i) - 3P_{\alpha\beta}(Y_i) - 3P_{\beta\gamma}(Y_i) - 3P_{\alpha\beta\gamma}(Y_i) - P_{\beta\gamma\delta}(Y_i) - P_{\alpha\beta\gamma\delta}(Y_i)
\end{aligned} \tag{2.2}$$

and

$$\begin{aligned}
&P_{(\alpha)}(Y_i) + 3P_{(\beta)}(Y_i) + 3P_{(\alpha\beta)}(Y_i) + 3P_{(\beta\gamma)}(Y_i) + 3P_{(\alpha\beta\gamma)}(Y_i) \\
&\quad + P_{(\beta\gamma\delta)}(Y_i) + P_{(\alpha\beta\gamma\delta)}(Y_i) \\
&= (1 - 3p_i)P_\alpha(Y_i) + 3p_iP_\beta(Y_i) + 3(1 - p_i)P_\beta(Y_i) + 3p_iP_\alpha(Y_i) \\
&\quad + 3(1 - 2p_i)P_{\alpha\beta}(Y_i) + 6p_iP_{\beta\gamma}(Y_i) + 3(1 - 2p_i)P_{\beta\gamma}(Y_i) + 6p_iP_{\alpha\beta}(Y_i) \\
&\quad + 3(1 - p_i)P_{\alpha\beta\gamma}(Y_i) + 3p_iP_{\beta\gamma\delta}(Y_i) + (1 - 3p_i)P_{\beta\gamma\delta}(Y_i) \\
&\quad + 3p_iP_{\alpha\beta\gamma}(Y_i) + P_{\alpha\beta\gamma\delta}(Y_i) \\
&\quad \text{by (8), (9), (10), (11), (12), (13), (14)} \\
&= P_\alpha(Y_i) + 3P_\beta(Y_i) + 3P_{\alpha\beta}(Y_i) + 3P_{\beta\gamma}(Y_i) + 3P_{\alpha\beta\gamma}(Y_i) + P_{\beta\gamma\delta}(Y_i) + P_{\alpha\beta\gamma\delta}(Y_i) \\
&= 1.
\end{aligned} \tag{2.3}$$

Furthermore, the following expressions can be simplified by (6), (2.2) and (2.3).

$$\begin{aligned}
&4P_{(\alpha)}(Y_i) + 6P_{(\alpha\beta)}(Y_i) + 4P_{(\alpha\beta\gamma)}(Y_i) + P_{(\alpha\beta\gamma\delta)}(Y_i) \\
&= 4\left(P_{(\alpha)}(Y_i) + \frac{3}{2}P_{(\alpha\beta)}(Y_i) + P_{(\alpha\beta\gamma)}(Y_i) + \frac{1}{4}P_{(\alpha\beta\gamma\delta)}(Y_i)\right) \\
&= 4\left((1 - 3p_i)P_\alpha(Y_i) + 3p_iP_\beta(Y_i)\right) + \frac{3}{2}\left((1 - 2p_i)P_{\alpha\beta}(Y_i) + 2p_iP_{\beta\gamma}(Y_i)\right) \\
&\quad + (1 - p_i)P_{\alpha\beta\gamma}(Y_i) + p_iP_{\beta\gamma\delta}(Y_i) + \frac{1}{4}P_{\alpha\beta\gamma\delta}(Y_i) \\
&= 4\left((1 - 3p_i)P_\alpha(Y_i) + p_i(1 - P_\alpha(Y_i) - 3P_{\alpha\beta}(Y_i) - 3P_{\beta\gamma}(Y_i) - 3P_{\alpha\beta\gamma}(Y_i) - P_{\beta\gamma\delta}(Y_i) - P_{\alpha\beta\gamma\delta}(Y_i))\right) \\
&\quad + \frac{3}{2}\left((1 - 2p_i)P_{\alpha\beta}(Y_i) + 2p_iP_{\beta\gamma}(Y_i)\right) + (1 - p_i)P_{\alpha\beta\gamma}(Y_i) + p_iP_{\beta\gamma\delta}(Y_i) + \frac{1}{4}P_{\alpha\beta\gamma\delta}(Y_i) \\
&\text{by (2.2)} \\
&= 4\left((1 - 3p_i)P_\alpha(Y_i) + p_i - p_iP_\alpha(Y_i) - 3p_iP_{\alpha\beta}(Y_i) - 3p_iP_{\beta\gamma}(Y_i) - 3p_iP_{\alpha\beta\gamma}(Y_i) - p_iP_{\beta\gamma\delta}(Y_i)\right) \\
&\quad - p_iP_{\alpha\beta\gamma\delta}(Y_i) + \frac{3}{2}\left((1 - 2p_i)P_{\alpha\beta}(Y_i) + 2p_iP_{\beta\gamma}(Y_i)\right) + (1 - p_i)P_{\alpha\beta\gamma}(Y_i) + p_iP_{\beta\gamma\delta}(Y_i) + \frac{1}{4}P_{\alpha\beta\gamma\delta}(Y_i) \\
&= 4\left((1 - 3p_i)P_\alpha(Y_i) + p_i - p_iP_\alpha(Y_i) - 3p_iP_{\alpha\beta}(Y_i) - 3p_iP_{\alpha\beta\gamma}(Y_i)\right) \\
&\quad - p_iP_{\alpha\beta\gamma\delta}(Y_i) + \frac{3}{2}\left(1 - 2p_i)P_{\alpha\beta}(Y_i) + (1 - p_i)P_{\alpha\beta\gamma}(Y_i) + \frac{1}{4}P_{\alpha\beta\gamma\delta}(Y_i)\right) \\
&= 4\left(p_i + (1 - 4p_i)P_\alpha(Y_i) + \frac{3}{2}(1 - 4p_i)P_{\alpha\beta}(Y_i) + (1 - 4p_i)P_{\alpha\beta\gamma}(Y_i) + \frac{1}{4}(1 - 4p_i)P_{\alpha\beta\gamma\delta}(Y_i)\right) \\
&= 4\left(p_i + (1 - 4p_i)\left(P_\alpha(Y_i) + \frac{3}{2}P_{\alpha\beta}(Y_i) + P_{\alpha\beta\gamma}(Y_i) + \frac{1}{4}P_{\alpha\beta\gamma\delta}(Y_i)\right)\right) \\
&= 4\left(p_i + (1 - 4p_i)RA(Y_i)\right)
\end{aligned} \tag{2.4}$$

by (6).

Moreover,

$$\begin{aligned}
& \frac{1}{2}P_{(\alpha)}(Y_i) + \frac{3}{2}P_{(\alpha\beta)}(Y_i) + \frac{3}{2}P_{(\alpha\beta\gamma)}(Y_i) + P_{(\alpha\beta\gamma\delta)}(Y_i) + \frac{3}{2}P_{(\beta)}(Y_i) + P_{(\beta\gamma)}(Y_i) + \frac{1}{4}P_{(\beta\gamma\delta)}(Y_i) \\
&= \frac{1}{2}P_{(\alpha)}(Y_i) + \frac{3}{2}P_{(\beta)}(Y_i) + \frac{3}{2}P_{(\alpha\beta)}(Y_i) + \frac{3}{2}P_{(\beta\gamma)}(Y_i) - \frac{1}{2}P_{(\beta\gamma)}(Y_i) + \frac{3}{2}P_{(\alpha\beta\gamma)}(Y_i) \\
&\quad + \frac{1}{2}P_{(\beta\gamma\delta)}(Y_i) - \frac{1}{4}P_{(\beta\gamma\delta)}(Y_i) + \frac{1}{2}P_{(\alpha\beta\gamma\delta)}(Y_i) + \frac{1}{2}P_{(\alpha\beta\gamma\delta)}(Y_i) \\
&= \frac{1}{2}\left(P_{(\alpha)}(Y_i) + 3P_{(\beta)}(Y_i) + 3P_{(\alpha\beta)}(Y_i) + 3P_{(\beta\gamma)}(Y_i) + 3P_{(\alpha\beta\gamma)}(Y_i) + P_{(\beta\gamma\delta)}(Y_i) + P_{(\alpha\beta\gamma\delta)}(Y_i)\right) \\
&\quad - \frac{1}{2}P_{(\beta\gamma)}(Y_i) - \frac{1}{4}P_{(\beta\gamma\delta)}(Y_i) + \frac{1}{2}P_{(\alpha\beta\gamma\delta)}(Y_i) \\
&= \frac{1}{2} - \frac{1}{2}P_{(\beta\gamma)}(Y_i) - \frac{1}{4}P_{(\beta\gamma\delta)}(Y_i) + \frac{1}{2}P_{(\alpha\beta\gamma\delta)}(Y_i) \\
&\quad \text{by (2.3)}.
\end{aligned} \tag{2.5}$$

Additionally,

$$\begin{aligned}
& \frac{3}{2}P_{(\alpha)}(Y_i) + 2P_{(\beta)}(Y_i) + \frac{15}{4}P_{(\alpha\beta)}(Y_i) + \frac{3}{4}P_{(\beta\gamma)}(Y_i) + 3P_{(\alpha\beta\gamma)}(Y_i) + \frac{3}{2}P_{(\alpha\beta\gamma\delta)}(Y_i) \\
&= \frac{2}{3}\left(P_{(\alpha)}(Y_i) + 3P_{(\beta)}(Y_i) + 3P_{(\alpha\beta)}(Y_i) + 3P_{(\beta\gamma)}(Y_i) + 3P_{(\alpha\beta\gamma)}(Y_i) + P_{(\beta\gamma\delta)}(Y_i) + P_{(\alpha\beta\gamma\delta)}(Y_i)\right) \\
&\quad + \frac{5}{6}P_{(\alpha)}(Y_i) + \frac{7}{4}P_{(\alpha\beta)}(Y_i) - \frac{5}{4}P_{(\beta\gamma)}(Y_i) + P_{(\alpha\beta\gamma)}(Y_i) - \frac{2}{3}P_{(\beta\gamma\delta)}(Y_i) + \frac{5}{6}P_{(\alpha\beta\gamma\delta)}(Y_i) \\
&= \frac{2}{3} + \frac{5}{6}P_{(\alpha)}(Y_i) + \frac{7}{4}P_{(\alpha\beta)}(Y_i) - \frac{5}{4}P_{(\beta\gamma)}(Y_i) + P_{(\alpha\beta\gamma)}(Y_i) - \frac{2}{3}P_{(\beta\gamma\delta)}(Y_i) + \frac{5}{6}P_{(\alpha\beta\gamma\delta)}(Y_i) \\
&\quad \text{by (2.3)},
\end{aligned} \tag{2.6}$$

and

$$\begin{aligned}
& \frac{3}{2}P_{(\alpha)}(Y_i) + \frac{3}{4}P_{(\beta)}(Y_i) + 3P_{(\alpha\beta)}(Y_i) + 2P_{(\alpha\beta\gamma)}(Y_i) + P_{(\alpha\beta\gamma\delta)}(Y_i) \\
&= \frac{1}{4}\left(P_{(\alpha)}(Y_i) + 3P_{(\beta)}(Y_i) + 3P_{(\alpha\beta)}(Y_i) + 3P_{(\beta\gamma)}(Y_i) + 3P_{(\alpha\beta\gamma)}(Y_i) + P_{(\beta\gamma\delta)}(Y_i) + P_{(\alpha\beta\gamma\delta)}(Y_i)\right) \\
&\quad + \frac{5}{4}P_{(\alpha)}(Y_i) + \frac{9}{4}P_{(\alpha\beta)}(Y_i) - \frac{3}{4}P_{(\beta\gamma)}(Y_i) + \frac{5}{4}P_{(\alpha\beta\gamma)}(Y_i) - \frac{1}{4}P_{(\beta\gamma\delta)}(Y_i) + \frac{3}{4}P_{(\alpha\beta\gamma\delta)}(Y_i) \\
&= \frac{1}{4} + \frac{5}{4}P_{(\alpha)}(Y_i) + \frac{9}{4}P_{(\alpha\beta)}(Y_i) - \frac{3}{4}P_{(\beta\gamma)}(Y_i) + \frac{5}{4}P_{(\alpha\beta\gamma)}(Y_i) - \frac{1}{4}P_{(\beta\gamma\delta)}(Y_i) + \frac{3}{4}P_{(\alpha\beta\gamma\delta)}(Y_i) \\
&\quad \text{by (2.3)}.
\end{aligned} \tag{2.7}$$

Furthermore,

$$\begin{aligned}
4p_i - 1 &= 4p_i - 4 + 3 + 12p - 12p \\
&= 3 - 12p + 4p_i - 4 + 12(p_i + p'_i - 4p_i p'_i) \\
&\quad \text{by (3)} \\
&= 3(1 - 4p) + 16p_i - 4 + 12p'_i - 48p_i p'_i \\
&= 3(1 - 4p) + 4(1 - 4p_i)(-1 + 3p'_i) \\
&= 3P + 4P_i(-1 + 3p'_i). \\
&\quad \text{by the definition of } P \text{ and } P_i,
\end{aligned} \tag{2.8}$$

and

$$\begin{aligned}
4p_i - 4 + 12p &= 4p_i - 4 + 12(p_i + p'_i - 4p_i p'_i) \\
&\quad \text{by (3)} \\
&= 4(4p_i - 1 + 3p'_i - 12p_i p'_i) \\
&= 4(1 - 4p_i)(-1 + 3p'_i) \\
&= 4P_i(-1 + 3p'_i) \\
&\quad \text{by the definition of } P_i.
\end{aligned} \tag{2.9}$$

By using the simplifications stated before we can now rewrite $RA(X)$.

$$\begin{aligned}
& RA(X) \\
&= P_\alpha(X) + \frac{3}{2} \cdot P_{\alpha\beta}(X) + P_{\alpha\beta\gamma}(X) + \frac{1}{4} \cdot P_{\alpha\beta\gamma\delta}(X) \\
&\text{by (6)} \\
&= P_{(\alpha)}(Y_1)P_{(\alpha)}(Y_2) + 3P_{(\alpha)}(Y_1)P_{(\alpha\beta)}(Y_2) + 3P_{(\alpha\beta)}(Y_1)P_{(\alpha)}(Y_2) \\
&\quad + 3P_{(\alpha)}(Y_1)P_{(\alpha\beta\gamma)}(Y_2) + 3P_{(\alpha\beta\gamma)}(Y_1)P_{(\alpha)}(Y_2) + 6P_{(\alpha\beta)}(Y_1)P_{(\alpha\beta)}(Y_2) \\
&\quad + 3P_{(\alpha\beta)}(Y_1)P_{(\alpha\beta\gamma)}(Y_2) + 3P_{(\alpha\beta\gamma)}(Y_1)P_{(\alpha\beta)}(Y_2) + P_{(\alpha)}(Y_1)P_{(\alpha\beta\gamma\delta)}(Y_2) \\
&\quad + P_{(\alpha\beta\gamma\delta)}(Y_1)P_{(\alpha)}(Y_2) + \frac{3}{2} \left(P_{(\alpha)}(Y_1)P_{(\beta)}(Y_2) + P_{(\beta)}(Y_1)P_{(\alpha)}(Y_2) \right. \\
&\quad + P_{(\alpha\beta)}(Y_1)P_{(\alpha\beta)}(Y_2) + 2P_{(\alpha\beta)}(Y_1)P_{(\alpha\beta\gamma)}(Y_2) + 2P_{(\alpha\beta\gamma)}(Y_1)P_{(\alpha\beta)}(Y_2) \\
&\quad + P_{(\alpha\beta)}(Y_1)P_{(\alpha\beta\gamma\delta)}(Y_2) + P_{(\alpha\beta\gamma\delta)}(Y_1)P_{(\alpha\beta)}(Y_2) + 2P_{(\alpha\beta\gamma)}(Y_1)P_{(\alpha\beta\gamma)}(Y_2) \left. \right) \\
&\quad + P_{(\alpha)}(Y_1)P_{(\beta\gamma)}(Y_2) + P_{(\beta\gamma)}(Y_1)P_{(\alpha)}(Y_2) + 2P_{(\beta)}(Y_1)P_{(\alpha\beta)}(Y_2) \\
&\quad + 2P_{(\alpha\beta)}(Y_1)P_{(\beta)}(Y_2) + P_{(\alpha\beta\gamma)}(Y_1)P_{(\alpha\beta\gamma)}(Y_2) + P_{(\alpha\beta\gamma)}(Y_1)P_{(\alpha\beta\gamma\delta)}(Y_2) \\
&\quad + P_{(\alpha\beta\gamma\delta)}(Y_1)P_{(\alpha\beta\gamma)}(Y_2) + \frac{1}{4} \left(P_{(\alpha)}(Y_1)P_{(\beta\gamma\delta)}(Y_2) + P_{(\beta\gamma\delta)}(Y_1)P_{(\alpha)}(Y_2) \right. \\
&\quad + 3P_{(\beta)}(Y_1)P_{(\alpha\beta\gamma)}(Y_2) + 3P_{(\alpha\beta\gamma)}(Y_1)P_{(\beta)}(Y_2) + 3P_{(\alpha\beta)}(Y_1)P_{(\beta\gamma)}(Y_2) \\
&\quad \left. + 3P_{(\beta\gamma)}(Y_1)P_{(\alpha\beta)}(Y_2) + P_{(\alpha\beta\gamma\delta)}(Y_1)P_{(\alpha\beta\gamma\delta)}(Y_2) \right) \\
&\text{by (15), (16), (17), (18)} \\
&= P_{(\alpha)}(Y_1) \left(\frac{1}{2}P_{(\alpha)}(Y_2) + \frac{3}{2}P_{(\alpha\beta)}(Y_2) + \frac{3}{2}P_{(\alpha\beta\gamma)}(Y_2) + P_{(\alpha\beta\gamma\delta)}(Y_2) + \frac{3}{2}P_{(\beta)}(Y_2) + P_{(\beta\gamma)}(Y_2) \right. \\
&\quad \left. + \frac{1}{4}P_{(\beta\gamma\delta)}(Y_2) \right) \\
&\quad + P_{(\alpha)}(Y_2) \left(\frac{1}{2}P_{(\alpha)}(Y_1) + \frac{3}{2}P_{(\alpha\beta)}(Y_1) + \frac{3}{2}P_{(\alpha\beta\gamma)}(Y_1) + P_{(\alpha\beta\gamma\delta)}(Y_1) + \frac{3}{2}P_{(\beta)}(Y_1) + P_{(\beta\gamma)}(Y_1) \right. \\
&\quad \left. + \frac{1}{4}P_{(\beta\gamma\delta)}(Y_1) \right) \\
&\quad + P_{(\alpha\beta)}(Y_1) \left(\frac{3}{2}P_{(\alpha)}(Y_2) + 2P_{(\beta)}(Y_2) + \frac{15}{4}P_{(\alpha\beta)}(Y_2) + \frac{3}{4}P_{(\beta\gamma)}(Y_2) + 3P_{(\alpha\beta\gamma)}(Y_2) + \frac{3}{2}P_{(\alpha\beta\gamma\delta)}(Y_2) \right) \\
&\quad + P_{(\alpha\beta)}(Y_2) \left(\frac{3}{2}P_{(\alpha)}(Y_1) + 2P_{(\beta)}(Y_1) + \frac{15}{4}P_{(\alpha\beta)}(Y_1) + \frac{3}{4}P_{(\beta\gamma)}(Y_1) + 3P_{(\alpha\beta\gamma)}(Y_1) + \frac{3}{2}P_{(\alpha\beta\gamma\delta)}(Y_1) \right) \\
&\quad + P_{(\alpha\beta\gamma)}(Y_1) \left(\frac{3}{2}P_{(\alpha)}(Y_2) + \frac{3}{4}P_{(\beta)}(Y_2) + 3P_{(\alpha\beta)}(Y_2) + 2P_{(\alpha\beta\gamma)}(Y_2) + P_{(\alpha\beta\gamma\delta)}(Y_2) \right) \\
&\quad + P_{(\alpha\beta\gamma)}(Y_2) \left(\frac{3}{2}P_{(\alpha)}(Y_1) + \frac{3}{4}P_{(\beta)}(Y_1) + 3P_{(\alpha\beta)}(Y_1) + 2P_{(\alpha\beta\gamma)}(Y_1) + P_{(\alpha\beta\gamma\delta)}(Y_1) \right) \\
&\quad + \frac{1}{4}P_{(\alpha\beta\gamma\delta)}(Y_1)P_{(\alpha\beta\gamma\delta)}(Y_2) \\
&= P_{(\alpha)}(Y_1) \left(\frac{1}{2} - \frac{1}{2}P_{(\beta\gamma)}(Y_2) - \frac{1}{4}P_{(\beta\gamma\delta)}(Y_2) + \frac{1}{2}P_{(\alpha\beta\gamma\delta)}(Y_2) \right) \\
&\quad + P_{(\alpha)}(Y_2) \left(\frac{1}{2} - \frac{1}{2}P_{(\beta\gamma)}(Y_1) - \frac{1}{4}P_{(\beta\gamma\delta)}(Y_1) + \frac{1}{2}P_{(\alpha\beta\gamma\delta)}(Y_1) \right) \\
&\quad + P_{(\alpha\beta)}(Y_1) \left(\frac{2}{3} + \frac{5}{6}P_{(\alpha)}(Y_2) + \frac{7}{4}P_{(\alpha\beta)}(Y_2) - \frac{5}{4}P_{(\beta\gamma)}(Y_2) + P_{(\alpha\beta\gamma)}(Y_2) - \frac{2}{3}P_{(\beta\gamma\delta)}(Y_2) + \frac{5}{6}P_{(\alpha\beta\gamma\delta)}(Y_2) \right) \\
&\quad + P_{(\alpha\beta)}(Y_2) \left(\frac{2}{3} + \frac{5}{6}P_{(\alpha)}(Y_1) + \frac{7}{4}P_{(\alpha\beta)}(Y_1) - \frac{5}{4}P_{(\beta\gamma)}(Y_1) + P_{(\alpha\beta\gamma)}(Y_1) - \frac{2}{3}P_{(\beta\gamma\delta)}(Y_1) + \frac{5}{6}P_{(\alpha\beta\gamma\delta)}(Y_1) \right) \\
&\quad + P_{(\alpha\beta\gamma)}(Y_1) \left(\frac{1}{4} + \frac{5}{4}P_{(\alpha)}(Y_2) + \frac{9}{4}P_{(\alpha\beta)}(Y_2) - \frac{3}{4}P_{(\beta\gamma)}(Y_2) + \frac{5}{4}P_{(\alpha\beta\gamma)}(Y_2) - \frac{1}{4}P_{(\beta\gamma\delta)}(Y_2) + \frac{3}{4}P_{(\alpha\beta\gamma\delta)}(Y_2) \right) \\
&\quad + P_{(\alpha\beta\gamma)}(Y_2) \left(\frac{1}{4} + \frac{5}{4}P_{(\alpha)}(Y_1) + \frac{9}{4}P_{(\alpha\beta)}(Y_1) - \frac{3}{4}P_{(\beta\gamma)}(Y_1) + \frac{5}{4}P_{(\alpha\beta\gamma)}(Y_1) - \frac{1}{4}P_{(\beta\gamma\delta)}(Y_1) + \frac{3}{4}P_{(\alpha\beta\gamma\delta)}(Y_1) \right) \\
&\quad + \frac{1}{4}P_{(\alpha\beta\gamma\delta)}(Y_1)P_{(\alpha\beta\gamma\delta)}(Y_2) \\
&\text{by (2.5), (2.6), (2.7)}
\end{aligned}$$

$$\begin{aligned}
&= \left(\frac{1}{2}P_{(\alpha)}(Y_1) + \frac{5}{4}P_{(\alpha\beta)}(Y_1) + \frac{3}{4}P_{(\alpha\beta\gamma)}(Y_1) \right) \left(P_{(\alpha\beta)}(Y_2) - P_{(\beta\gamma)}(Y_2) \right) \\
&\quad + \left(\frac{1}{2}P_{(\alpha)}(Y_2) + \frac{5}{4}P_{(\alpha\beta)}(Y_2) + \frac{3}{4}P_{(\alpha\beta\gamma)}(Y_2) \right) \left(P_{(\alpha\beta)}(Y_1) - P_{(\beta\gamma)}(Y_1) \right) \\
&\quad + \left(\frac{1}{4}P_{(\alpha)}(Y_1) + \frac{2}{3}P_{(\alpha\beta)}(Y_1) + \frac{1}{4}P_{(\alpha\beta\gamma)}(Y_1) \right) \left(P_{(\alpha\beta\gamma)}(Y_2) - P_{(\beta\gamma\delta)}(Y_2) \right) \\
&\quad + \left(\frac{1}{4}P_{(\alpha)}(Y_2) + \frac{2}{3}P_{(\alpha\beta)}(Y_2) + \frac{1}{4}P_{(\alpha\beta\gamma)}(Y_2) \right) \left(P_{(\alpha\beta\gamma)}(Y_1) - P_{(\beta\gamma\delta)}(Y_1) \right) \\
&\quad + \frac{1}{2} \left(p_1 + P_1RA(Y_1) \right) + \frac{1}{2} \left(p_2 + P_2RA(Y_2) \right) \\
&\quad + \left(\frac{1}{12}P_{(\alpha\beta)}(Y_1) + \frac{1}{4}P_{(\alpha\beta\gamma)}(Y_1) + \frac{1}{8}P_{(\alpha\beta\gamma\delta)}(Y_1) \right) \left(-1 + 4 \left(p_2 + P_2RA(Y_2) \right) \right) \\
&\quad + \left(\frac{1}{12}P_{(\alpha\beta)}(Y_2) + \frac{1}{4}P_{(\alpha\beta\gamma)}(Y_2) + \frac{1}{8}P_{(\alpha\beta\gamma\delta)}(Y_2) \right) \left(-1 + 4 \left(p_1 + P_1RA(Y_1) \right) \right) \\
&\text{by the definition of } P_1 \text{ and } P_2
\end{aligned}$$

Then

$$\begin{aligned}
8D(X) &= 8RA(X) - 8 + 24p \\
&= \left(4P_{(\alpha)}(Y_1) + 10P_{(\alpha\beta)}(Y_1) + 6P_{(\alpha\beta\gamma)}(Y_1) \right) \left(P_{(\alpha\beta)}(Y_2) - P_{(\beta\gamma)}(Y_2) \right) \\
&\quad + \left(4P_{(\alpha)}(Y_2) + 10P_{(\alpha\beta)}(Y_2) + 6P_{(\alpha\beta\gamma)}(Y_2) \right) \left(P_{(\alpha\beta)}(Y_1) - P_{(\beta\gamma)}(Y_1) \right) \\
&\quad + \left(2P_{(\alpha)}(Y_1) + \frac{16}{3}P_{(\alpha\beta)}(Y_1) + 2P_{(\alpha\beta\gamma)}(Y_1) \right) \left(P_{(\alpha\beta\gamma)}(Y_2) - P_{(\beta\gamma\delta)}(Y_2) \right) \\
&\quad + \left(2P_{(\alpha)}(Y_2) + \frac{16}{3}P_{(\alpha\beta)}(Y_2) + 2P_{(\alpha\beta\gamma)}(Y_2) \right) \left(P_{(\alpha\beta\gamma)}(Y_1) - P_{(\beta\gamma\delta)}(Y_1) \right) \\
&\quad + 4p_1 + 4P_1RA(Y_1) - 4 + 12p + 4p_2 + 4P_2RA(Y_2) - 4 + 12p \\
&\quad + \left(\frac{2}{3}P_{(\alpha\beta)}(Y_1) + 2P_{(\alpha\beta\gamma)}(Y_1) + P_{(\alpha\beta\gamma\delta)}(Y_1) \right) \left(-1 + 4p_2 + 4P_2RA(Y_2) \right) \\
&\quad + \left(\frac{2}{3}P_{(\alpha\beta)}(Y_2) + 2P_{(\alpha\beta\gamma)}(Y_2) + P_{(\alpha\beta\gamma\delta)}(Y_2) \right) \left(-1 + 4p_1 + 4P_1RA(Y_1) \right) \\
&= \left(4P_{(\alpha)}(Y_1) + 10P_{(\alpha\beta)}(Y_1) + 6P_{(\alpha\beta\gamma)}(Y_1) \right) \left(P_{(\alpha\beta)}(Y_2) - P_{(\beta\gamma)}(Y_2) \right) \\
&\quad + \left(4P_{(\alpha)}(Y_2) + 10P_{(\alpha\beta)}(Y_2) + 6P_{(\alpha\beta\gamma)}(Y_2) \right) \left(P_{(\alpha\beta)}(Y_1) - P_{(\beta\gamma)}(Y_1) \right) \\
&\quad + \left(2P_{(\alpha)}(Y_1) + \frac{16}{3}P_{(\alpha\beta)}(Y_1) + 2P_{(\alpha\beta\gamma)}(Y_1) \right) \left(P_{(\alpha\beta\gamma)}(Y_2) - P_{(\beta\gamma\delta)}(Y_2) \right) \\
&\quad + \left(2P_{(\alpha)}(Y_2) + \frac{16}{3}P_{(\alpha\beta)}(Y_2) + 2P_{(\alpha\beta\gamma)}(Y_2) \right) \left(P_{(\alpha\beta\gamma)}(Y_1) - P_{(\beta\gamma\delta)}(Y_1) \right) \\
&\quad + 4P_1RA(Y_1) + 4P_1(-1 + 3p'_1) + 4P_2RA(Y_2) + 4P_2(-1 + 3p'_2) \\
&\quad + \left(\frac{2}{3}P_{(\alpha\beta)}(Y_1) + 2P_{(\alpha\beta\gamma)}(Y_1) + P_{(\alpha\beta\gamma\delta)}(Y_1) \right) \left(3P + 4P_2(-1 + 3p'_2) + 4P_2RA(Y_2) \right) \\
&\quad + \left(\frac{2}{3}P_{(\alpha\beta)}(Y_2) + 2P_{(\alpha\beta\gamma)}(Y_2) + P_{(\alpha\beta\gamma\delta)}(Y_2) \right) \left(3P + 4P_1(-1 + 3p'_1) + 4P_1RA(Y_1) \right) \\
&\text{by (2.8), (2.9)} \\
&= \left(4P_{(\alpha)}(Y_1) + 10P_{(\alpha\beta)}(Y_1) + 6P_{(\alpha\beta\gamma)}(Y_1) \right) \left(P_{(\alpha\beta)}(Y_2) - P_{(\beta\gamma)}(Y_2) \right) \\
&\quad + \left(4P_{(\alpha)}(Y_2) + 10P_{(\alpha\beta)}(Y_2) + 6P_{(\alpha\beta\gamma)}(Y_2) \right) \left(P_{(\alpha\beta)}(Y_1) - P_{(\beta\gamma)}(Y_1) \right) \\
&\quad + \left(2P_{(\alpha)}(Y_1) + \frac{16}{3}P_{(\alpha\beta)}(Y_1) + 2P_{(\alpha\beta\gamma)}(Y_1) \right) \left(P_{(\alpha\beta\gamma)}(Y_2) - P_{(\beta\gamma\delta)}(Y_2) \right) \\
&\quad + \left(2P_{(\alpha)}(Y_2) + \frac{16}{3}P_{(\alpha\beta)}(Y_2) + 2P_{(\alpha\beta\gamma)}(Y_2) \right) \left(P_{(\alpha\beta\gamma)}(Y_1) - P_{(\beta\gamma\delta)}(Y_1) \right) \\
&\quad + 4P_1(RA(Y_1) - 1 + 3p'_1) + 4P_2(RA(Y_2) - 1 + 3p'_2) \\
&\quad + \left(\frac{2}{3}P_{(\alpha\beta)}(Y_1) + 2P_{(\alpha\beta\gamma)}(Y_1) + P_{(\alpha\beta\gamma\delta)}(Y_1) \right) \left(3P + 4P_2(-1 + 3p'_2 + RA(Y_2)) \right) \\
&\quad + \left(\frac{2}{3}P_{(\alpha\beta)}(Y_2) + 2P_{(\alpha\beta\gamma)}(Y_2) + P_{(\alpha\beta\gamma\delta)}(Y_2) \right) \left(3P + 4P_1(-1 + 3p'_1 + RA(Y_1)) \right)
\end{aligned}$$

$$\begin{aligned}
&= \left(4P_{(\alpha)}(Y_1) + 10P_{(\alpha\beta)}(Y_1) + 6P_{(\alpha\beta\gamma)}(Y_1)\right) \left(P_{(\alpha\beta)}(Y_2) - P_{(\beta\gamma)}(Y_2)\right) \\
&\quad + \left(4P_{(\alpha)}(Y_2) + 10P_{(\alpha\beta)}(Y_2) + 6P_{(\alpha\beta\gamma)}(Y_2)\right) \left(P_{(\alpha\beta)}(Y_1) - P_{(\beta\gamma)}(Y_1)\right) \\
&\quad + \left(2P_{(\alpha)}(Y_1) + \frac{16}{3}P_{(\alpha\beta)}(Y_1) + 2P_{(\alpha\beta\gamma)}(Y_1)\right) \left(P_{(\alpha\beta\gamma)}(Y_2) - P_{(\beta\gamma\delta)}(Y_2)\right) \\
&\quad + \left(2P_{(\alpha)}(Y_2) + \frac{16}{3}P_{(\alpha\beta)}(Y_2) + 2P_{(\alpha\beta\gamma)}(Y_2)\right) \left(P_{(\alpha\beta\gamma)}(Y_1) - P_{(\beta\gamma\delta)}(Y_1)\right) \\
&\quad + 4P_1D_1 + 4P_2D_2 \\
&\quad + \left(\frac{2}{3}P_{(\alpha\beta)}(Y_1) + 2P_{(\alpha\beta\gamma)}(Y_1) + P_{(\alpha\beta\gamma\delta)}(Y_1)\right) \left(3P + 4P_2D_2\right) \\
&\quad + \left(\frac{2}{3}P_{(\alpha\beta)}(Y_2) + 2P_{(\alpha\beta\gamma)}(Y_2) + P_{(\alpha\beta\gamma\delta)}(Y_2)\right) \left(3P + 4P_1D_1\right) \\
&\text{by the definition of } D_1, D_2 \\
&= \left(4P_{(\alpha)}(Y_1) + 10P_{(\alpha\beta)}(Y_1) + 6P_{(\alpha\beta\gamma)}(Y_1)\right) \left(P_{\alpha\beta}(Y_2) - P_{\beta\gamma}(Y_2)\right) P_2 \\
&\quad + \left(4P_{(\alpha)}(Y_2) + 10P_{(\alpha\beta)}(Y_2) + 6P_{(\alpha\beta\gamma)}(Y_2)\right) \left(P_{\alpha\beta}(Y_1) - P_{\beta\gamma}(Y_1)\right) P_1 \\
&\quad + \left(2P_{(\alpha)}(Y_1) + \frac{16}{3}P_{(\alpha\beta)}(Y_1) + 2P_{(\alpha\beta\gamma)}(Y_1)\right) \left(P_{\alpha\beta\gamma}(Y_2) - P_{\beta\gamma\delta}(Y_2)\right) P_2 \\
&\quad + \left(2P_{(\alpha)}(Y_2) + \frac{16}{3}P_{(\alpha\beta)}(Y_2) + 2P_{(\alpha\beta\gamma)}(Y_2)\right) \left(P_{\alpha\beta\gamma}(Y_1) - P_{\beta\gamma\delta}(Y_1)\right) P_1 \\
&\quad + 4P_1D_1 + 4P_2D_2 \\
&\quad + \left(\frac{2}{3}P_{(\alpha\beta)}(Y_1) + 2P_{(\alpha\beta\gamma)}(Y_1) + P_{(\alpha\beta\gamma\delta)}(Y_1)\right) \left(3P + 4P_2D_2\right) \\
&\quad + \left(\frac{2}{3}P_{(\alpha\beta)}(Y_2) + 2P_{(\alpha\beta\gamma)}(Y_2) + P_{(\alpha\beta\gamma\delta)}(Y_2)\right) \left(3P + 4P_1D_1\right) \\
&\text{by (1.9), (1.10)}
\end{aligned}$$

3 Proof of Lemma 2

To prove Lemma 2 we show that for any rooted binary phylogenetic tree T under a symmetric 3-state substitution model

$$P_{\alpha}(X) \geq P_{\beta}(X), \quad (3.1)$$

$$P_{\alpha\beta}(X) \geq P_{\beta\gamma}(X), \quad (3.2)$$

by induction on n . For $n = 2$ the subtrees Y_1 and Y_2 both contain one leaf, which leads to

$$\begin{aligned}
P_{\alpha}(X) &= (1 - 2p_1)(1 - 2p_2), \\
P_{\beta}(X) &= p_1p_2, \\
P_{\alpha\beta}(X) &= (1 - 2p_1)p_2 + p_1(1 - 2p_2), \\
P_{\beta\gamma}(X) &= 2p_1p_2.
\end{aligned}$$

Therefore

$$\begin{aligned}
P_{\alpha}(X) - P_{\beta}(X) &= (1 - 2p_1)(1 - 2p_2) - p_1p_2 = 1 - 2p_1 - 2p_2 + 4p_1p_2 - p_1p_2 = 1 - 2p_1 - 2p_2 + 3p_1p_2 \\
&= \underbrace{(1 - 3p_1)}_{\geq 0} \underbrace{(1 - 3p_2)}_{\geq 0} + p_1 \underbrace{(1 - 3p_2)}_{\geq 0} + \underbrace{(1 - 3p_1)}_{\geq 0} p_2 \geq 0 \text{ as } 0 \leq p_1, p_2 \leq \frac{1}{3}.
\end{aligned}$$

Moreover

$$P_{\alpha\beta}(X) - P_{\beta\gamma}(X) = (1 - 2p_1)p_2 + p_1(1 - 2p_2) - 2p_1p_2 = \underbrace{(1 - 3p_1)}_{\geq 0} p_2 + p_1 \underbrace{(1 - 3p_2)}_{\geq 0} \geq 0 \text{ as } 0 \leq p_1, p_2 \leq \frac{1}{3},$$

which completes the base case of the induction. For the inductive step we first define some recursions similar to (8), (9), (10), (11) and (12):

$$P_{(\alpha)}(Y_i) = (1 - 2p_i)P_\alpha(Y_i) + 2p_iP_\beta(Y_i), \quad (3.3)$$

$$P_{(\beta)}(Y_i) = (1 - p_i)P_\beta(Y_i) + p_iP_\alpha(Y_i) = P_{(\gamma)}(Y_i), \quad (3.4)$$

$$P_{(\alpha\beta)}(Y_i) = (1 - p_i)P_{\alpha\beta}(Y_i) + p_iP_{\beta\gamma}(Y_i) = P_{(\alpha\gamma)}(Y_i), \quad (3.5)$$

$$P_{(\beta\gamma)}(Y_i) = (1 - 2p_i)P_{\beta\gamma}(Y_i) + 2p_iP_{\alpha\beta}(Y_i), \quad (3.6)$$

$$P_{(\alpha\beta\gamma)}(Y_i) = P_{\alpha\beta\gamma}(Y_i), \quad (3.7)$$

With (3.3), (3.4), (3.5), (3.6) and (3.7) we therefore have:

$$\begin{aligned} P_\alpha(X) &= P_{(\alpha)}(Y_1)P_{(\alpha)}(Y_2) + 2P_{(\alpha)}(Y_1)P_{(\alpha\beta)}(Y_2) + 2P_{(\alpha\beta)}(Y_1)P_{(\alpha)}(Y_2) \\ &\quad + 2P_{(\alpha\beta)}(Y_1)P_{(\alpha\beta)}(Y_2) + P_{(\alpha)}(Y_1)P_{(\alpha\beta\gamma)}(Y_2) + P_{(\alpha\beta\gamma)}(Y_1)P_{(\alpha)}(Y_2) \end{aligned} \quad (3.8)$$

$$\begin{aligned} P_\beta(X) &= P_{(\beta)}(Y_1)P_{(\beta)}(Y_2) + P_{(\beta)}(Y_1)P_{(\alpha\beta)}(Y_2) + P_{(\alpha\beta)}(Y_1)P_{(\beta)}(Y_2) \\ &\quad + P_{(\beta)}(Y_1)P_{(\beta\gamma)}(Y_2) + P_{(\beta\gamma)}(Y_1)P_{(\beta)}(Y_2) + P_{(\alpha\beta)}(Y_1)P_{(\beta\gamma)}(Y_2) \\ &\quad + P_{(\beta\gamma)}(Y_1)P_{(\alpha\beta)}(Y_2) + P_{(\beta)}(Y_1)P_{(\alpha\beta\gamma)}(Y_2) + P_{(\alpha\beta\gamma)}(Y_1)P_{(\beta)}(Y_2) \end{aligned} \quad (3.9)$$

$$\begin{aligned} P_{\alpha\beta}(X) &= P_{(\alpha)}(Y_1)P_{(\beta)}(Y_2) + P_{(\beta)}(Y_1)P_{(\alpha)}(Y_2) + P_{(\alpha\beta)}(Y_1)P_{(\alpha\beta)}(Y_2) \\ &\quad + P_{(\alpha\beta)}(Y_1)P_{(\alpha\beta\gamma)}(Y_2) + P_{(\alpha\beta\gamma)}(Y_1)P_{(\alpha\beta)}(Y_2) \end{aligned} \quad (3.10)$$

$$\begin{aligned} P_{\beta\gamma}(X) &= 2P_{(\beta)}(Y_1)P_{(\beta)}(Y_2) + P_{(\beta\gamma)}(Y_1)P_{(\beta\gamma)}(Y_2) \\ &\quad + P_{(\beta\gamma)}(Y_1)P_{(\alpha\beta\gamma)}(Y_2) + P_{(\alpha\beta\gamma)}(Y_1)P_{(\beta\gamma)}(Y_2) \end{aligned} \quad (3.11)$$

Moreover we have that for $i \in \{1, 2\}$

$$\begin{aligned} P_{(\alpha)}(Y_i) - P_{(\beta)}(Y_i) &= (1 - 2p_i)P_\alpha(Y_i) + 2p_iP_\beta(Y_i) - (1 - p_i)P_\beta(Y_i) - p_iP_\alpha(Y_i) \\ &\quad \text{by (3.3), (3.4)} \\ &= (1 - 3p_i)P_\alpha(Y_i) - (1 - 3p_i)P_\beta(Y_i) \\ &= (1 - 3p_i)\left(P_\alpha(Y_i) - P_\beta(Y_i)\right) \end{aligned} \quad (3.12)$$

and thus

$$P_{(\alpha)}(Y_i) = P_{(\beta)}(Y_i) + (1 - 3p_i)\left(P_\alpha(Y_i) - P_\beta(Y_i)\right). \quad (3.13)$$

In the same manner by (3.5) and (3.6) we can see that

$$P_{(\alpha\beta)}(Y_i) - P_{(\beta\gamma)}(Y_i) = (1 - 3p_i)\left(P_{\alpha\beta}(Y_i) - P_{\beta\gamma}(Y_i)\right), \quad (3.14)$$

Therefore

$$P_{(\alpha\beta)}(Y_i) = P_{(\beta\gamma)}(Y_i) + (1 - 3p_i)\left(P_{\alpha\beta}(Y_i) - P_{\beta\gamma}(Y_i)\right). \quad (3.15)$$

Additionally we have the following: choose sets A_1, A_2 from $\{\{\alpha\}, \{\alpha\beta\}\}$ and B_1, B_2 from $\{\{\beta\}, \{\beta\gamma\}\}$ such that for $i \in \{1, 2\}$ $|A_i| = |B_i|$, respectively. Then we have that

$$\begin{aligned} &P_{(A_1)}(Y_1)P_{(A_2)}(Y_2) - P_{(B_1)}(Y_1)P_{(B_2)}(Y_2) \\ &= \left(P_{(B_1)}(Y_1) + (1 - 3p_1)\left(P_{A_1}(Y_1) - P_{B_1}(Y_1)\right)\right)\left(P_{(B_2)}(Y_2) + (1 - 3p_2)\left(P_{A_2}(Y_2) - P_{B_2}(Y_2)\right)\right) \\ &\quad - P_{(B_1)}(Y_1)P_{(B_2)}(Y_2) \\ &\quad \text{by (3.13) or (3.15)} \\ &= P_{(B_1)}(Y_1)P_{(B_2)}(Y_2) \\ &\quad + P_{(B_1)}(Y_1)(1 - 3p_2)\left(P_{A_2}(Y_2) - P_{B_2}(Y_2)\right) + P_{(B_2)}(Y_2)(1 - 3p_1)\left(P_{A_1}(Y_1) - P_{B_1}(Y_1)\right) \\ &\quad + (1 - 3p_1)(1 - 3p_2)\left(P_{A_1}(Y_1) - P_{B_1}(Y_1)\right)\left(P_{A_2}(Y_2) - P_{B_2}(Y_2)\right) - P_{(B_1)}(Y_1)P_{(B_2)}(Y_2) \\ &= P_{(B_1)}(Y_1)(1 - 3p_2)\left(P_{A_2}(Y_2) - P_{B_2}(Y_2)\right) + P_{(B_2)}(Y_2)(1 - 3p_1)\left(P_{A_1}(Y_1) - P_{B_1}(Y_1)\right) \\ &\quad + (1 - 3p_1)(1 - 3p_2)\left(P_{A_1}(Y_1) - P_{B_1}(Y_1)\right)\left(P_{A_2}(Y_2) - P_{B_2}(Y_2)\right). \end{aligned} \quad (3.16)$$

Now suppose that T has n taxa and that (3.1) and (3.2) are true for all trees having fewer than n taxa. Note that therefore (3.16) is non-negative, since Y_1 and Y_2 contain both fewer than n taxa. Then

$$\begin{aligned}
& P_\alpha(X) - P_\beta(X) \\
&= P_{(\alpha)}(Y_1)P_{(\alpha)}(Y_2) + 2P_{(\alpha)}(Y_1)P_{(\alpha\beta)}(Y_2) + 2P_{(\alpha\beta)}(Y_1)P_{(\alpha)}(Y_2) \\
&\quad + 2P_{(\alpha\beta)}(Y_1)P_{(\alpha\beta)}(Y_2) + P_{(\alpha)}(Y_1)P_{(\alpha\beta\gamma)}(Y_2) + P_{(\alpha\beta\gamma)}(Y_1)P_{(\alpha)}(Y_2) \\
&\quad - P_{(\beta)}(Y_1)P_{(\beta)}(Y_2) - P_{(\beta)}(Y_1)P_{(\alpha\beta)}(Y_2) - P_{(\alpha\beta)}(Y_1)P_{(\beta)}(Y_2) \\
&\quad - P_{(\beta)}(Y_1)P_{(\beta\gamma)}(Y_2) - P_{(\beta\gamma)}(Y_1)P_{(\beta)}(Y_2) - P_{(\alpha\beta)}(Y_1) \cdot P_{(\beta\gamma)}(Y_2) \\
&\quad - P_{(\beta\gamma)}(Y_1)P_{(\alpha\beta)}(Y_2) - P_{(\beta)}(Y_1)P_{(\alpha\beta\gamma)}(Y_2) - P_{(\alpha\beta\gamma)}(Y_1)P_{(\beta)}(Y_2) \\
&= P_{(\alpha)}(Y_1)P_{(\alpha)}(Y_2) - P_{(\beta)}(Y_1)P_{(\beta)}(Y_2) \\
&\quad + P_{(\alpha\beta)}(Y_2)\left(P_{(\alpha)}(Y_1) - P_{(\beta)}(Y_1)\right) + P_{(\alpha\beta)}(Y_1)\left(P_{(\alpha)}(Y_2) - P_{(\beta)}(Y_2)\right) \\
&\quad + P_{(\alpha)}(Y_1)P_{(\alpha\beta)}(Y_2) - P_{(\beta)}(Y_1)P_{(\beta\gamma)}(Y_2) \\
&\quad + P_{(\alpha\beta)}(Y_1)P_{(\alpha)}(Y_2) - P_{(\beta\gamma)}(Y_1)P_{(\beta)}(Y_2) \\
&\quad + P_{(\alpha\beta)}(Y_2)\left(P_{(\alpha\beta)}(Y_1) - P_{(\beta\gamma)}(Y_1)\right) + P_{(\alpha\beta)}(Y_1)\left(P_{(\alpha\beta)}(Y_2) - P_{(\beta\gamma)}(Y_2)\right) \\
&\quad + P_{(\alpha\beta\gamma)}(Y_2)\left(P_{(\alpha)}(Y_1) - P_{(\beta)}(Y_1)\right) + P_{(\alpha\beta\gamma)}(Y_1)\left(P_{(\alpha)}(Y_2) - P_{(\beta)}(Y_2)\right) \\
&= P_{(\beta)}(Y_1)(1 - 3p_2)\left(P_\alpha(Y_2) - P_\beta(Y_2)\right) + P_{(\beta)}(Y_2)(1 - 3p_1)\left(P_\alpha(Y_1) - P_\beta(Y_1)\right) \\
&\quad + (1 - 3p_1)(1 - 3p_2)\left(P_\alpha(Y_1) - P_\beta(Y_1)\right)\left(P_\alpha(Y_2) - P_\beta(Y_2)\right) \\
&\quad + P_{(\alpha\beta)}(Y_2)(1 - 3p_1)\left(P_\alpha(Y_1) - P_\beta(Y_1)\right) + P_{(\alpha\beta)}(Y_1)(1 - 3p_2)\left(P_\alpha(Y_2) - P_\beta(Y_2)\right) \\
&\quad + P_{(\beta)}(Y_1)(1 - 3p_2)\left(P_{\alpha\beta}(Y_2) - P_{\beta\gamma}(Y_2)\right) + P_{(\beta\gamma)}(Y_2)(1 - 3p_1)\left(P_\alpha(Y_1) - P_\beta(Y_1)\right) \\
&\quad + (1 - 3p_1)(1 - 3p_2)\left(P_\alpha(Y_1) - P_\beta(Y_1)\right)\left(P_{\alpha\beta}(Y_2) - P_{\beta\gamma}(Y_2)\right) \\
&\quad + P_{(\beta\gamma)}(Y_1)(1 - 3p_2)\left(P_\alpha(Y_2) - P_\beta(Y_2)\right) + P_{(\beta)}(Y_2)(1 - 3p_1)\left(P_{\alpha\beta}(Y_1) - P_{\beta\gamma}(Y_1)\right) \\
&\quad + (1 - 3p_1)(1 - 3p_2)\left(P_{\alpha\beta}(Y_1) - P_{\beta\gamma}(Y_1)\right)\left(P_\alpha(Y_2) - P_\beta(Y_2)\right) \\
&\quad + P_{(\alpha\beta)}(Y_2)(1 - 3p_1)\left(P_{\alpha\beta}(Y_1) - P_{\beta\gamma}(Y_1)\right) + P_{(\alpha\beta)}(Y_1)(1 - 3p_2)\left(P_{\alpha\beta}(Y_2) - P_{\beta\gamma}(Y_2)\right) \\
&\quad + P_{(\alpha\beta\gamma)}(Y_2)(1 - 3p_1)\left(P_\alpha(Y_1) - P_\beta(Y_1)\right) + P_{(\alpha\beta\gamma)}(Y_1)(1 - 3p_2)\left(P_\alpha(Y_2) - P_\beta(Y_2)\right) \\
&\text{by (3.12), (3.14), (3.16)}
\end{aligned}$$

By the inductive assumption this term is non-negative, and therefore concludes the proof for $P_\alpha(X) \geq P_\beta(X)$. We now proceed with the second part of Lemma 2.

$$\begin{aligned}
& P_{\alpha\beta}(X) - P_{\beta\gamma}(X) \\
&= P_{(\alpha)}(Y_1)P_{(\beta)}(Y_2) + P_{(\beta)}(Y_1)P_{(\alpha)}(Y_2) + P_{(\alpha\beta)}(Y_1)P_{(\alpha\beta)}(Y_2) \\
&\quad + P_{(\alpha\beta)}(Y_1)P_{(\alpha\beta\gamma)}(Y_2) + P_{(\alpha\beta\gamma)}(Y_1)P_{(\alpha\beta)}(Y_2) - 2P_{(\beta)}(Y_1)P_{(\beta)}(Y_2) \\
&\quad - P_{(\beta\gamma)}(Y_1)P_{(\beta\gamma)}(Y_2) - P_{(\beta\gamma)}(Y_1)P_{(\alpha\beta\gamma)}(Y_2) - P_{(\alpha\beta\gamma)}(Y_1)P_{(\beta\gamma)}(Y_2) \\
&= P_{(\beta)}(Y_2)\left(P_{(\alpha)}(Y_1) - P_{(\beta)}(Y_1)\right) + P_{(\beta)}(Y_1)\left(P_{(\alpha)}(Y_2) - P_{(\beta)}(Y_2)\right) \\
&\quad + P_{(\alpha\beta)}(Y_1)P_{(\alpha\beta)}(Y_2) - P_{(\beta\gamma)}(Y_1)P_{(\beta\gamma)}(Y_2) \\
&\quad + P_{(\alpha\beta\gamma)}(Y_2)\left(P_{(\alpha\beta)}(Y_1) - P_{(\beta\gamma)}(Y_1)\right) + P_{(\alpha\beta\gamma)}(Y_1)\left(P_{(\alpha\beta)}(Y_2) - P_{(\beta\gamma)}(Y_2)\right) \\
&= P_{(\beta)}(Y_2)(1 - 3p_1)\left(P_\alpha(Y_1) - P_\beta(Y_1)\right) + P_{(\beta)}(Y_1)(1 - 3p_2)\left(P_\alpha(Y_2) - P_\beta(Y_2)\right) \\
&\quad + P_{(\beta\gamma)}(Y_1)(1 - 3p_2)\left(P_{\alpha\beta}(Y_2) - P_{\beta\gamma}(Y_2)\right) + P_{(\beta\gamma)}(Y_2)(1 - 3p_1)\left(P_{\alpha\beta}(Y_1) - P_{\beta\gamma}(Y_1)\right) \\
&\quad + (1 - 3p_1)(1 - 3p_2)\left(P_{\alpha\beta}(Y_1) - P_{\beta\gamma}(Y_1)\right)\left(P_{\alpha\beta}(Y_2) - P_{\beta\gamma}(Y_2)\right) \\
&\quad + P_{(\alpha\beta\gamma)}(Y_2)(1 - 3p_1)\left(P_{\alpha\beta}(Y_1) - P_{\beta\gamma}(Y_1)\right) + P_{(\alpha\beta\gamma)}(Y_1)(1 - 3p_2)\left(P_{\alpha\beta}(Y_2) - P_{\beta\gamma}(Y_2)\right) \\
&\text{by (3.12), (3.14), (3.16)}
\end{aligned}$$

By inductive assumption $P_{\alpha\beta}(X) - P_{\beta\gamma}(X)$ is non-negative, and therefore concludes the proof of the second part of Lemma 2. \square