Supplementary Material for "CMPLE: Correlation modelling to decode Photosynthesis using the Minorize-Maximize algorithm"

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Appendix

A.1 Photosynthetic model and Electron transfer chain

Under ideal conditions, a large fraction of solar energy is used to drive photochemical reactions. This fraction is usually termed the quantum yield of photochemistry. Productive photochemistry induces a series of electron and proton transfer reactions, resulting in the formation of biochemical energy-storing products, ATP and NADPH, which in turn are used to drive the fixation of CO_2 and other cellular processes . These electron transfers involve two chlorophyll-containing complexes, Photosystem I (PS I) and Photosystem II (PS II), which are essentially connected by the cytochrome b6f complex and mobile electron carriers plastoquinone/plastoquinol (PQ/PQH2) and plastocyanin (PC). In "non-cyclic photophosphorylation", PS II oxidizes the water and releases protons into the lumen, which travels down an electron transport chain to PSI while forming an electrochemical proton gradient (pmf, proton motive force) and passes to NADP+ to make NADPH (Figure 1).

Under different abiotic stresses, plants regulate their photosynthetic machinary by triggering various nonphotochemical quenching processes (NPQ). Process (A) (Energydependent NPQ (qE)) activated by acidification of the thylakoid lumen resulting in quenching excitation energy through the qE mechanism. This is reflected by the positive correlation between $NPQt$ and $ECSt$. On the other hand, formation of reactive oxygen species can damage PS II, resulting in Process (B) (long-lived photoinhibition-related NPQ (qI)) and decrease the number of active PS II centers which can be observed by the negative correlation between $NPQt$ and $ECSt$. These two processes are illustrated in the Figure 2. It is noteworthy that these two forms of NPQ are both induced under conditions where light input exceeds capacity and have similar effects on photochemical efficiency.

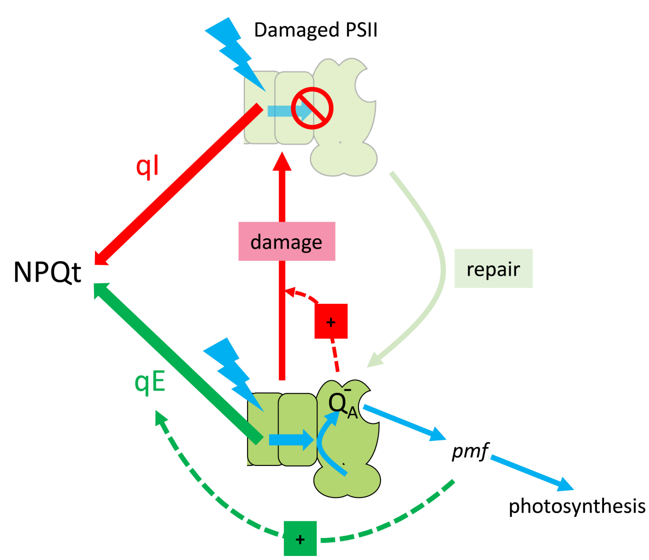

Figure 1: Simplified schematics for regulating light energy capture and storage by plant photosynthesis

However, the qE form is typically considered to act as a primary photoprotective mechanism and is readily reversed. In contrast, the qI form involves protein damage, the repair of which requires degradation and resynthesis of the PS II D1 protein, and is thus considered to reflect more severe responses (Raven, 2011). This patterns are highly influenced by a number of other factors as well. Kramer et al. (2003) showed that at under lower CO_2 and increasing light, there is a rapid drop in the yield of PS II (ϕ_{II}) and a corresponding rapid rise in the yield of NPQ, together with a decrease in qL. But, under high CO_2 there is a slower drop in the yield of PS II and qL with increasing light, and slower rise in the yield of NPQ. This shows that multiple parts of the photosynthetic machinery indulges in co-regulating the quenching behaviours.

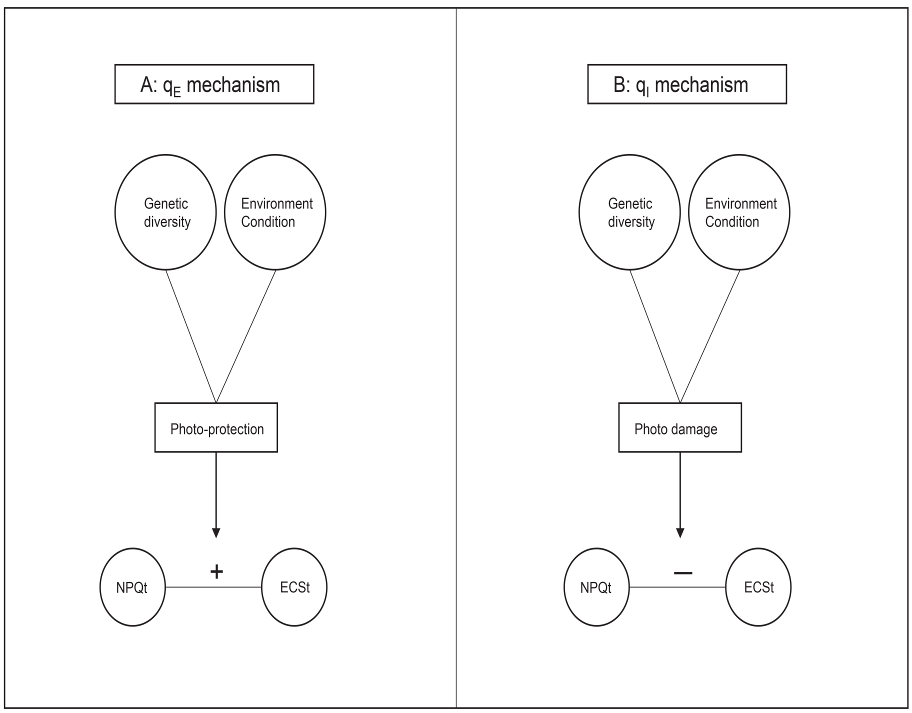

Figure 2: Flowchart of photo-protection and photo-damage through purely correlative scheme

A.2 Proof of Theorem 1

Conditional on the covariate $\boldsymbol{X}_i$, $\boldsymbol{Y}_i = (Y_{i,1}, \ldots, Y_{i,q})^T$ follows a multivariate normal distribution with mean 0 and variance-covariance matrix $\boldsymbol{\Sigma}_i$. As defined in Section 3.1, the pairwise likelihood for the (j,k)th response is $\mathcal{L}_{j,k}(\boldsymbol{\theta}) = \prod_{i=1}^n f(Y_{i,j}, Y_{i,k}|\boldsymbol{X}_i)$, with $f(Y_{i,j}, Y_{i,k}|\boldsymbol{X}_i)$ is given in (4). The logarithm of $\mathcal{L}_{j,k}(\boldsymbol{\theta})$ is

$$\ell_{j,k}(\boldsymbol{\alpha}, \boldsymbol{\delta}) = -\frac{1}{2}\sum_{i=1}^n \left[\log(\sigma_{i,j}^2) + \log(\sigma_{i,k}^2) + \log(1-\rho_{i,j,k}^2) + \frac{1}{(1-\rho_{i,j,k}^2)}\left(\frac{Y_{i,j}^2}{\sigma_{i,j}^2} - \frac{2\rho_{i,j,k}Y_{i,j}Y_{i,k}}{\sigma_{i,j}\sigma_{i,k}} + \frac{Y_{i,k}^2}{\sigma_{i,k}^2}\right)\right].$$

To derive the minorization function for $\ell_{j,k}$, we consider each term separately. Consider the following term

$$\begin{aligned}
-\frac{Y_{i,j}^2}{\sigma_{i,j}^2(1-\rho_{i,j,k}^2)} &= -\frac{Y_{i,j}^2}{\sigma_{i,j}^{(0)^2}(1-\rho_{i,j,k}^{(0)^2})} \times \frac{\sigma_{i,j}^{(0)^2}(1-\rho_{i,j,k}^{(0)^2})}{\sigma_{i,j}^2(1-\rho_{i,j,k}^2)} \\
&\geq -\frac{Y_{i,j}^2}{2\sigma_{i,j}^{(0)^2}(1-\rho_{i,j,k}^{(0)^2})}\left\{\left(\frac{\sigma_{i,j}^{(0)}}{\sigma_{i,j}}\right)^4 + \left(\frac{1-\rho_{i,j,k}^{(0)^2}}{1-\rho_{i,j,k}^2}\right)^2\right\}.
\end{aligned}$$

The above inequality follows from the AM-GM inequality. Similarly, we have

$$\begin{aligned}
-\frac{Y_{i,k}^2}{\sigma_{i,k}^2(1-\rho_{i,j,k}^2)} &= -\frac{Y_{i,k}^2}{\sigma_{i,k}^{(0)^2}(1-\rho_{i,j,k}^{(0)^2})} \times \frac{\sigma_{i,k}^{(0)^2}(1-\rho_{i,j,k}^{(0)^2})}{\sigma_{i,k}^2(1-\rho_{i,j,k}^2)} \\
&\geq -\frac{Y_{i,k}^2}{2\sigma_{i,k}^{(0)^2}(1-\rho_{i,j,k}^{(0)^2})}\left\{\left(\frac{\sigma_{i,k}^{(0)}}{\sigma_{i,k}}\right)^4 + \left(\frac{1-\rho_{i,j,k}^{(0)^2}}{1-\rho_{i,j,k}^2}\right)^2\right\}.
\end{aligned}$$

Next, after replacing $\rho_{i,j,k}$ by $1-2/\{1+\exp(\delta_{j,k,0}+\sum_{r=1}^p \delta_{j,k,r}X_{i,r})\}$ in the term $\rho_{i,j,k}Y_{i,j}Y_{i,k}/\sigma_{i,j}\sigma_{i,k}(1-\rho_{i,j,k}^2)$ we obtain

$$\begin{aligned}
\frac{\rho_{i,j,k}Y_{i,j}Y_{i,k}}{\sigma_{i,j}\sigma_{i,k}(1-\rho_{i,j,k}^2)} &= \frac{Y_{i,j}Y_{i,k}}{\sigma_{i,j}\sigma_{i,k}(1-\rho_{i,j,k}^2)} - \frac{2Y_{i,j}Y_{i,k}}{\sigma_{i,j}\sigma_{i,k}(1-\rho_{i,j,k}^2)\{1+\exp(\delta_{j,k,0}+\sum_{r=1}^p \delta_{j,k,r}X_{i,r})\}} \\
&= \frac{\left(Y_{i,j}+Y_{i,k}\right)^2 - \left(Y_{i,j}^2+Y_{i,k}^2\right)}{2\sigma_{i,j}\sigma_{i,k}(1-\rho_{i,j,k}^2)} \\
&\quad - \frac{\left(Y_{i,j}+Y_{i,k}\right)^2 - \left(Y_{i,j}^2+Y_{i,k}^2\right)}{\sigma_{i,j}\sigma_{i,k}(1-\rho_{i,j,k}^2)\{1+\exp(\delta_{j,k,0}+\sum_{r=1}^p \delta_{j,k,r}X_{i,r})\}} \qquad \text{(A.1)} \\
&= B_1 + B_2 + B_3 + B_4.
\end{aligned}$$

Now,

$$B_1 = \frac{\left(Y_{i,j}+Y_{i,k}\right)^2}{2\sigma_{i,j}\sigma_{i,k}(1-\rho_{i,j,k}^2)} \geq \frac{\left(Y_{i,j}+Y_{i,k}\right)^2}{2\sigma_{i,j}^{(0)}\sigma_{i,k}^{(0)}(1-\rho_{i,j,k}^{(0)^2})}\left\{1+\log\left(\frac{\sigma_{i,j}^{(0)}}{\sigma_{i,j}}\right)+\left(\frac{\sigma_{i,k}^{(0)}}{\sigma_{i,k}}\right)+\left(\frac{1-\rho_{i,j,k}^{(0)^2}}{1-\rho_{i,j,k}^2}\right)\right\},$$

and this inequality follows due to the fact that for any generic $x>0$, $x \geq \{1+\log(x)\}$ and equality holds when $x=1$. Next, using the AM-GM inequality we have

$$B_2 = -\frac{\left(Y_{i,j}^2+Y_{i,k}^2\right)}{2\sigma_{i,j}\sigma_{i,k}(1-\rho_{i,j,k}^2)} \geq -\frac{\left(Y_{i,j}^2+Y_{i,k}^2\right)}{6\sigma_{i,j}^{(0)}\sigma_{i,k}^{(0)}(1-\rho_{i,j,k}^{(0)^2})}\left\{\left(\frac{\sigma_{i,j}^{(0)}}{\sigma_{i,j}}\right)^3+\left(\frac{\sigma_{i,k}^{(0)}}{\sigma_{i,k}}\right)^3+\left(\frac{1-\rho_{i,j,k}^{(0)^2}}{1-\rho_{i,j,k}^2}\right)^3\right\}.$$

After replacing $1+\exp(\delta_{j,k,0}+\sum_{r=1}^{p}\delta_{j,k,r}X_{i,r})$ by $2/\left(1-\rho_{i,j,k}\right)$ in (A.1), we have

$$B_3+B_4 = -\frac{\left(Y_{i,j}+Y_{i,k}\right)^2}{2\sigma_{i,j}\sigma_{i,k}(1+\rho_{i,j,k})}+\frac{\left(Y_{i,j}^2+Y_{i,k}^2\right)}{2\sigma_{i,j}\sigma_{i,k}(1+\rho_{i,j,k})}.$$

Now,

$$\begin{aligned} B_3 &= -\frac{\left(Y_{i,j}+Y_{i,k}\right)^2}{2\sigma_{i,j}\sigma_{i,k}(1+\rho_{i,j,k})} \\ &\geq -\frac{\left(Y_{i,j}+Y_{i,k}\right)^2}{6\sigma_{i,j}^{(0)}\sigma_{i,k}^{(0)}(1+\rho_{i,j,k}^{(0)})}\left\{\left(\frac{\sigma_{i,j}^{(0)}}{\sigma_{i,j}}\right)^3+\left(\frac{\sigma_{i,k}^{(0)}}{\sigma_{i,k}}\right)^3+\left(\frac{1+\rho_{i,j,k}^{(0)}}{1+\rho_{i,j,k}}\right)^3\right\}, \end{aligned}$$

and

$$\begin{aligned} B_4 &= \frac{\left(Y_{i,j}^2+Y_{i,k}^2\right)}{2\sigma_{i,j}\sigma_{i,k}(1+\rho_{i,j,k})} \\ &\geq \frac{\left(Y_{i,j}^2+Y_{i,k}^2\right)}{2\sigma_{i,j}^{(0)}\sigma_{i,k}^{(0)}(1+\rho_{i,j,k}^{(0)})}\left\{1+\log\left(\frac{\sigma_{i,j}^{(0)}}{\sigma_{i,j}}\right)+\log\left(\frac{\sigma_{i,k}^{(0)}}{\sigma_{i,k}}\right)+\log\left(\frac{1+\rho_{i,j,k}^{(0)}}{1+\rho_{i,j,k}}\right)\right\}, \end{aligned}$$

and these two inequalities follow from the AM-GM inequality and $x \geq 1+\log(x)$ for any generic $x>0$.

We further define

$$\psi_{1,j,k}(\boldsymbol{\alpha}_r-\boldsymbol{\alpha}_r^{(0)}, r|\boldsymbol{\theta}^{(0)})$$

$$
\begin{aligned}
= & \sum_{i=1}^{n}\Bigg\{\log\left(\frac{\sigma_{i,r}^{(0)}}{\sigma_{i,r}}\right) - \frac{Y_{i,r}^2}{4\sigma_{i,r}^{(0)^2}(1-\rho_{i,j,k}^{(0)^2})}\left(\frac{\sigma_{i,r}^{(0)}}{\sigma_{i,r}}\right)^4 + \frac{\left(Y_{i,j}+Y_{i,k}\right)^2}{2\sigma_{i,j}^{(0)}\sigma_{i,k}^{(0)}(1-\rho_{i,j,k}^{(0)^2})}\log\left(\frac{\sigma_{i,r}^{(0)}}{\sigma_{i,r}}\right) \\
& - \frac{(Y_{i,j}^2+Y_{i,k}^2)}{6\sigma_{i,j}^{(0)}\sigma_{i,k}^{(0)}(1-\rho_{i,j,k}^{(0)^2})}\left(\frac{\sigma_{i,r}^{(0)}}{\sigma_{i,r}}\right)^3 - \frac{\left(Y_{i,j}+Y_{i,k}\right)^2}{6\sigma_{i,j}^{(0)}\sigma_{i,k}^{(0)}(1+\rho_{i,j,k}^{(0)})}\left(\frac{\sigma_{i,r}^{(0)}}{\sigma_{i,r}}\right)^3 \\
& + \frac{\left(Y_{i,j}^2+Y_{i,k}^2\right)}{2\sigma_{i,j}^{(0)}\sigma_{i,k}^{(0)}(1+\rho_{i,j,k}^{(0)})}\log\left(\frac{\sigma_{i,r}^{(0)}}{\sigma_{i,r}}\right)\Bigg\}, \\
= & \sum_{i=1}^{n}\Bigg[\boldsymbol{Z}_i^\top(\boldsymbol{\alpha}_r^{(0)}-\boldsymbol{\alpha}_r) - \frac{Y_{i,r}^2}{4\sigma_{i,r}^{(0)^2}(1-\rho_{i,j,k}^{(0)^2})}\exp\{4\boldsymbol{Z}_i^\top(\boldsymbol{\alpha}_r^{(0)}-\boldsymbol{\alpha}_r)\} \\
& + \frac{\left(Y_{i,j}+Y_{i,k}\right)^2}{2\sigma_{i,j}^{(0)}\sigma_{i,k}^{(0)}(1-\rho_{i,j,k}^{(0)^2})}\boldsymbol{Z}_i^\top(\boldsymbol{\alpha}_r^{(0)}-\boldsymbol{\alpha}_r) \\
& - \Bigg\{\frac{(Y_{i,j}^2+Y_{i,k}^2)}{6\sigma_{i,j}^{(0)}\sigma_{i,k}^{(0)}(1-\rho_{i,j,k}^{(0)^2})} + \frac{\left(Y_{i,j}+Y_{i,k}\right)^2}{6\sigma_{i,j}^{(0)}\sigma_{i,k}^{(0)}(1+\rho_{i,j,k}^{(0)})}\Bigg\}\exp\{3\boldsymbol{Z}_i^\top(\boldsymbol{\alpha}_r^{(0)}-\boldsymbol{\alpha}_r)\} \\
& + \frac{\left(Y_{i,j}^2+Y_{i,k}^2\right)}{2\sigma_{i,j}^{(0)}\sigma_{i,k}^{(0)}(1+\rho_{i,j,k}^{(0)})}\boldsymbol{Z}_i^\top(\boldsymbol{\alpha}_r^{(0)}-\boldsymbol{\alpha}_r)\Bigg] \\
= & \sum_{i=1}^{n}\Bigg[\Bigg\{1 + \frac{\left(Y_{i,j}+Y_{i,k}\right)^2}{2\sigma_{i,j}^{(0)}\sigma_{i,k}^{(0)}(1-\rho_{i,j,k}^{(0)^2})} + \frac{\left(Y_{i,j}^2+Y_{i,k}^2\right)}{2\sigma_{i,j}^{(0)}\sigma_{i,k}^{(0)}(1+\rho_{i,j,k}^{(0)})}\Bigg\}\boldsymbol{Z}_i^\top(\boldsymbol{\alpha}_r^{(0)}-\boldsymbol{\alpha}_r) \\
& - \frac{Y_{i,r}^2}{4\sigma_{i,r}^{(0)^2}(1-\rho_{i,j,k}^{(0)^2})}\exp\{4\boldsymbol{Z}_i^\top(\boldsymbol{\alpha}_r^{(0)}-\boldsymbol{\alpha}_r)\} \\
& - \Bigg\{\frac{(Y_{i,j}^2+Y_{i,k}^2)}{6\sigma_{i,j}^{(0)}\sigma_{i,k}^{(0)}(1-\rho_{i,j,k}^{(0)^2})} + \frac{\left(Y_{i,j}+Y_{i,k}\right)^2}{6\sigma_{i,j}^{(0)}\sigma_{i,k}^{(0)}(1+\rho_{i,j,k}^{(0)})}\Bigg\}\exp\{3\boldsymbol{Z}_i^\top(\boldsymbol{\alpha}_r^{(0)}-\boldsymbol{\alpha}_r)\}\Bigg],
\end{aligned}
$$

$$
\begin{aligned}
\psi_{2,j,k}(\rho_{j,k}|\boldsymbol{\theta}^{(0)}) = & \sum_{i=1}^{n}\Bigg[-\frac{1}{2}\log(1-\rho_{i,j,k}^2) - \Bigg\{\frac{Y_{i,j}^2}{4\sigma_{i,j}^{(0)^2}(1-\rho_{i,j,k}^{(0)^2})} + \frac{Y_{i,k}^2}{4\sigma_{i,k}^{(0)^2}(1-\rho_{i,j,k}^{(0)^2})}\Bigg\}\left(\frac{1-\rho_{i,j,k}^{(0)^2}}{1-\rho_{i,j,k}^2}\right)^2 \\
& + \frac{\left(Y_{i,j}+Y_{i,k}\right)^2}{2\sigma_{i,j}^{(0)}\sigma_{i,k}^{(0)}(1-\rho_{i,j,k}^{(0)^2})}\log\left(\frac{1-\rho_{i,j,k}^{(0)^2}}{1-\rho_{i,j,k}^2}\right)
\end{aligned}
$$

$$
- \frac{\left(Y_{i,j}^2 + Y_{i,k}^2\right)}{6\sigma_{i,j}^{(0)}\sigma_{i,k}^{(0)}(1-\rho_{i,j,k}^{(0)^2})} \left(\frac{1-\rho_{i,j,k}^{(0)^2}}{1-\rho_{i,j,k}^2}\right)^3 - \frac{\left(Y_{i,j} + Y_{i,k}\right)^2}{6\sigma_{i,j}^{(0)}\sigma_{i,k}^{(0)}(1+\rho_{i,j,k}^{(0)})} \left(\frac{1+\rho_{i,j,k}^{(0)}}{1+\rho_{i,j,k}}\right)^3
+ \frac{\left(Y_{i,j}^2 + Y_{i,k}^2\right)}{2\sigma_{i,j}^{(0)}\sigma_{i,k}^{(0)}(1+\rho_{i,j,k}^{(0)})} \log\left(\frac{1+\rho_{i,j,k}^{(0)}}{1+\rho_{i,j,k}}\right)\Bigg].
$$

Since $\rho_{i,j,k} = 1 - 2/\{1+\exp(\boldsymbol{\delta}_{j,k}^\top \boldsymbol{Z}_i)\}$, $1+\rho_{i,j,k} = 2\exp(\boldsymbol{\delta}_{j,k}^\top \boldsymbol{Z}_i)/\{1+\exp(\boldsymbol{\delta}_{j,k}^\top \boldsymbol{Z}_i)\}$, $\rho_{i,j,k}^2 = \{\exp(\boldsymbol{\delta}_{j,k}^\top \boldsymbol{Z}_i) - 1\}^2/\{\exp(\boldsymbol{\delta}_{j,k}^\top \boldsymbol{Z}_i)+1\}^2$, $1-\rho_{i,j,k}^2 = 4\exp(\boldsymbol{\delta}_{j,k}^\top \boldsymbol{Z}_i)/\{\exp(\boldsymbol{\delta}_{j,k}^\top \boldsymbol{Z}_i)+1\}^2$. Now using these terms, we obtain

$$
\begin{aligned}
\psi_{2,j,k}(\rho_{j,k}|\boldsymbol{\theta}^{(0)}) = \sum_{i=1}^n \Bigg(& -\frac{\log(4)}{2} - 0.5\boldsymbol{\delta}_{j,k}^\top \boldsymbol{Z}_i + \log\{\exp(\boldsymbol{\delta}_{j,k}^\top \boldsymbol{Z}_i)+1\} \\
& - \left(\frac{Y_{i,j}^2}{\sigma_{i,j}^{(0)^2}} + \frac{Y_{i,k}^2}{\sigma_{i,k}^{(0)^2}}\right)\left(1-\rho_{i,j,k}^{(0)^2}\right) \times \frac{\{\exp(\boldsymbol{\delta}_{j,k}^\top \boldsymbol{Z}_i)+1\}^4}{64\exp(2\boldsymbol{\delta}_{j,k}^\top \boldsymbol{Z}_i)} \\
& + \frac{\left(Y_{i,j}+Y_{i,k}\right)^2}{2\sigma_{i,j}^{(0)}\sigma_{i,k}^{(0)}(1-\rho_{i,j,k}^{(0)^2})}\left[\log\left(1-\rho_{i,j,k}^{(0)^2}\right) - \log(4) - \boldsymbol{\delta}_{j,k}^\top \boldsymbol{Z}_i + 2\log\{\exp(\boldsymbol{\delta}_{j,k}^\top \boldsymbol{Z}_i)+1\}\right] \\
& - \frac{\left(Y_{i,j}^2+Y_{i,k}^2\right)}{6\sigma_{i,j}^{(0)}\sigma_{i,k}^{(0)}}\left(1-\rho_{i,j,k}^{(0)^2}\right)^2 \times \frac{\{1+\exp(\boldsymbol{\delta}_{j,k}^\top \boldsymbol{Z}_i)\}^6}{64\exp(3\boldsymbol{\delta}_{j,k}^\top \boldsymbol{Z}_i)} \\
& - \frac{\left(Y_{i,j}+Y_{i,k}\right)^2}{6\sigma_{i,j}^{(0)}\sigma_{i,k}^{(0)}}\left(1+\rho_{i,j,k}^{(0)}\right)^2 \times \frac{\{1+\exp(\boldsymbol{\delta}_{j,k}^\top \boldsymbol{Z}_i)\}^3}{8\exp(3\boldsymbol{\delta}_{j,k}^\top \boldsymbol{Z}_i)} \\
& + \frac{\left(Y_{i,j}^2+Y_{i,k}^2\right)}{2\sigma_{i,j}^{(0)}\sigma_{i,k}^{(0)}(1+\rho_{i,j,k}^{(0)})}\left[\log\left(1+\rho_{i,j,k}^{(0)}\right) - \log(2) - \boldsymbol{\delta}_{j,k}^\top \boldsymbol{Z}_i + \log\{1+\exp(\boldsymbol{\delta}_{j,k}^\top \boldsymbol{Z}_i)\}\right]\Bigg).
\end{aligned}
$$

Also,

$$
\psi_{3,j,k}(\boldsymbol{\theta}^{(0)}) = \sum_{i=1}^n \left\{ \frac{\left(Y_{i,j}+Y_{i,k}\right)^2}{2\sigma_{i,j}^{(0)}\sigma_{i,k}^{(0)}(1-\rho_{i,j,k}^{(0)^2})} + \frac{\left(Y_{i,j}^2+Y_{i,k}^2\right)}{2\sigma_{i,j}^{(0)}\sigma_{i,k}^{(0)}(1+\rho_{i,j,k}^{(0)})} - \frac{1}{2}\log(\sigma_{i,j}^{(0)^2}\sigma_{i,k}^{(0)^2}) \right\}.
$$

Now, the minorization of the composite log-likelihood is

$$
\ell^*(\boldsymbol{\theta}|\boldsymbol{\theta}^{(0)}) = \sum_{j=1}^{(q-1)} \sum_{k=(j+1)}^{q} \Bigg\{ \psi_{1,j,k}(\boldsymbol{\alpha}_j - \boldsymbol{\alpha}_j^{(0)}, j|\boldsymbol{\theta}^{(0)}) + \psi_{1,j,k}(\boldsymbol{\alpha}_k - \boldsymbol{\alpha}_k^{(0)}, k|\boldsymbol{\theta}^{(0)})
$$

$$+\psi_{2,j,k}(\rho_{j,k}|\boldsymbol{\theta}^{(0)})+\psi_{3,j,k}(\boldsymbol{\theta}^{(0)})\Big\}$$

$$=\sum_{j=1}^{q} g_1(\boldsymbol{\alpha}_j|\boldsymbol{\theta}^{(0)})+\sum\sum_{j<k} g_2(\boldsymbol{\delta}_{j,k}|\boldsymbol{\theta}^{(0)})+g_3(\boldsymbol{\theta}^{(0)}),$$

where $g_1(\boldsymbol{\alpha}_j|\boldsymbol{\theta}^{(0)})=\sum_{s:s<j}\psi_{1,s,j}(\boldsymbol{\alpha}_j-\boldsymbol{\alpha}_j^{(0)},j|\boldsymbol{\theta}^{(0)})+\sum_{s:s>j}\psi_{1,j,s}(\boldsymbol{\alpha}_j-\boldsymbol{\alpha}_j^{(0)},j|\boldsymbol{\theta}^{(0)})$ for $j=1,\ldots,q$, $g_2(\boldsymbol{\delta}_{j,k}|\boldsymbol{\theta}^{(0)})=\psi_{2,j,k}(\rho_{j,k}|\boldsymbol{\theta}^{(0)})$ for $j\neq k$, $g_3(\boldsymbol{\theta}^{(0)})=\sum\sum_{j<k}\psi_{3,j,k}(\boldsymbol{\theta}^{(0)})$.

A.3 Detailed expression of the terms involved in Equation (4) of the manuscript

Observe that $\partial\ell^*(\boldsymbol{\theta}|\boldsymbol{\theta}^{(t)})/\partial\boldsymbol{\alpha}_j=\partial g_1(\boldsymbol{\alpha}_j|\boldsymbol{\theta}^{(t)})/\partial\boldsymbol{\alpha}_j=\sum_{s:s<j}\partial\psi_{1,s,j}(\boldsymbol{\alpha}_j-\boldsymbol{\alpha}_j^{(t)},j|\boldsymbol{\theta}^{(t)})/\partial\boldsymbol{\alpha}_j+\sum_{s:s>j}\partial\psi_{1,j,s}(\boldsymbol{\alpha}_j-\boldsymbol{\alpha}_j^{(t)},j|\boldsymbol{\theta}^{(t)})/\partial\boldsymbol{\alpha}_j$ for $j=1,\ldots,q$. Now,

$$\begin{aligned}\psi_{1,j,s}(\boldsymbol{\alpha}_j-\boldsymbol{\alpha}_j^{(0)},j|\boldsymbol{\theta}^{(0)})=\sum_{i=1}^{n}\Bigg[&\Bigg\{1+\frac{\Big(Y_{i,j}+Y_{i,s}\Big)^2}{2\sigma_{i,j}^{(0)}\sigma_{i,s}^{(0)}(1-\rho_{i,j,s}^{(0)2})}+\frac{\Big(Y_{i,j}^2+Y_{i,s}^2\Big)}{2\sigma_{i,j}^{(0)}\sigma_{i,s}^{(0)}(1+\rho_{i,j,s}^{(0)})}\Bigg\}\boldsymbol{Z}_i^\top(\boldsymbol{\alpha}_j^{(0)}-\boldsymbol{\alpha}_j)\\&-\frac{Y_{i,j}^2}{4\sigma_{i,j}^{(0)2}(1-\rho_{i,j,s}^{(0)2})}\exp\{4\boldsymbol{Z}_i^\top(\boldsymbol{\alpha}_j^{(0)}-\boldsymbol{\alpha}_j)\}\\&-\Bigg\{\frac{(Y_{i,j}^2+Y_{i,s}^2)}{6\sigma_{i,j}^{(0)}\sigma_{i,s}^{(0)}(1-\rho_{i,j,s}^{(0)2})}+\frac{\Big(Y_{i,j}+Y_{i,s}\Big)^2}{6\sigma_{i,j}^{(0)}\sigma_{i,s}^{(0)}(1+\rho_{i,j,s}^{(0)})}\Bigg\}\exp\{3\boldsymbol{Z}_i^\top(\boldsymbol{\alpha}_j^{(0)}-\boldsymbol{\alpha}_j)\}\Bigg],\end{aligned}$$

so

$$\begin{aligned}\frac{\partial\psi_{1,j,s}(\boldsymbol{\alpha}_j-\boldsymbol{\alpha}_j^{(0)},j|\boldsymbol{\theta}^{(0)})}{\partial\boldsymbol{\alpha}_j}=\sum_{i=1}^{n}\Bigg[&-\Bigg\{1+\frac{\Big(Y_{i,j}+Y_{i,s}\Big)^2}{2\sigma_{i,j}^{(0)}\sigma_{i,s}^{(0)}(1-\rho_{i,j,s}^{(0)2})}+\frac{\Big(Y_{i,j}^2+Y_{i,s}^2\Big)}{2\sigma_{i,j}^{(0)}\sigma_{i,s}^{(0)}(1+\rho_{i,j,s}^{(0)})}\Bigg\}\\&+\frac{Y_{i,j}^2}{\sigma_{i,j}^{(0)2}(1-\rho_{i,j,s}^{(0)2})}\exp\{4\boldsymbol{Z}_i^\top(\boldsymbol{\alpha}_j^{(0)}-\boldsymbol{\alpha}_j)\}\\&+\Bigg\{\frac{(Y_{i,j}^2+Y_{i,s}^2)}{2\sigma_{i,j}^{(0)}\sigma_{i,s}^{(0)}(1-\rho_{i,j,s}^{(0)2})}+\frac{\Big(Y_{i,j}+Y_{i,s}\Big)^2}{2\sigma_{i,j}^{(0)}\sigma_{i,s}^{(0)}(1+\rho_{i,j,s}^{(0)})}\Bigg\}\exp\{3\boldsymbol{Z}_i^\top(\boldsymbol{\alpha}_j^{(0)}-\boldsymbol{\alpha}_j)\}\Bigg]\boldsymbol{Z}_i,\end{aligned}$$

and

$$\left(\frac{\partial\psi_{1,j,s}(\boldsymbol{\alpha}_j-\boldsymbol{\alpha}_j^{(t)},j|\boldsymbol{\theta}^{(t)})}{\partial\boldsymbol{\alpha}_j}\right)_{\boldsymbol{\theta}=\boldsymbol{\theta}^{(t)}}=\sum_{i=1}^{n}\Bigg[-\Bigg\{1+\frac{\Big(Y_{i,j}+Y_{i,s}\Big)^2}{2\sigma_{i,j}^{(t)}\sigma_{i,s}^{(t)}(1-\rho_{i,j,s}^{(t)2})}+\frac{\Big(Y_{i,j}^2+Y_{i,s}^2\Big)}{2\sigma_{i,j}^{(t)}\sigma_{i,s}^{(t)}(1+\rho_{i,j,s}^{(t)})}\Bigg\}$$

$$+\frac{Y_{i,j}^2}{\sigma_{i,j}^{(t)^2}(1-\rho_{i,j,s}^{(t)^2})}+\left\{\frac{(Y_{i,j}^2+Y_{i,s}^2)}{2\sigma_{i,j}^{(t)}\sigma_{i,s}^{(t)}(1-\rho_{i,j,s}^{(t)^2})}+\frac{\left(Y_{i,j}+Y_{i,s}\right)^2}{2\sigma_{i,j}^{(t)}\sigma_{i,s}^{(t)}(1+\rho_{i,j,s}^{(t)})}\right\}\Bigg]\boldsymbol{Z}_i,$$
$$=\sum_{i=1}^{n}\Bigg\{-1+\frac{Y_{i,j}^2}{\sigma_{i,j}^{(t)^2}(1-\rho_{i,j,s}^{(t)^2})}-\frac{Y_{i,j}Y_{i,s}}{\sigma_{i,j}^{(t)}\sigma_{i,s}^{(t)}(1-\rho^{(t)}{}_{i,j,s}^2)}+\frac{Y_{i,j}Y_{i,s}}{\sigma_{i,j}^{(t)}\sigma_{i,s}^{(t)}(1+\rho_{i,j,s}^{(t)})}\Bigg\}\boldsymbol{Z}_i.$$

Likewise,

$$\left(\frac{\partial\psi_{1,s,j}(\boldsymbol{\alpha}_j-\boldsymbol{\alpha}_j^{(t)},j|\boldsymbol{\theta}^{(t)})}{\partial\boldsymbol{\alpha}_j}\right)_{\boldsymbol{\theta}=\boldsymbol{\theta}^{(t)}} = \sum_{i=1}^{n}\Bigg\{-1+\frac{Y_{i,j}^2}{\sigma_{i,j}^{(t)^2}(1-\rho_{i,s,j}^{(t)^2})}-\frac{Y_{i,j}Y_{i,s}}{\sigma_{i,j}^{(t)}\sigma_{i,s}^{(t)}(1-\rho^{(t)}{}_{i,s,j}^2)}+\frac{Y_{i,j}Y_{i,s}}{\sigma_{i,j}^{(t)}\sigma_{i,s}^{(t)}(1+\rho_{i,s,j}^{(t)})}\Bigg\}\boldsymbol{Z}_i.$$

Adding the above two expressions, we obtain

$$\left(\frac{\partial\ell^*(\boldsymbol{\theta}|\boldsymbol{\theta}^{(t)})}{\partial\boldsymbol{\alpha}_j}\right)_{\boldsymbol{\theta}=\boldsymbol{\theta}^{(t)}} = \sum_{s:s<j}\sum_{i=1}^{n}\Bigg\{-1+\frac{Y_{i,j}^2}{\sigma_{i,j}^{(t)^2}(1-\rho_{i,s,j}^{(t)^2})}-\frac{Y_{i,j}Y_{i,s}}{\sigma_{i,j}^{(t)}\sigma_{i,s}^{(t)}(1-\rho^{(t)}{}_{i,s,j}^2)}+\frac{Y_{i,j}Y_{i,s}}{\sigma_{i,j}^{(t)}\sigma_{i,s}^{(t)}(1+\rho_{i,s,j}^{(t)})}\Bigg\}\boldsymbol{Z}_i+\sum_{s:s>j}\sum_{i=1}^{n}\Bigg\{-1+\frac{Y_{i,j}^2}{\sigma_{i,j}^{(t)^2}(1-\rho_{i,j,s}^{(t)^2})}-\frac{Y_{i,j}Y_{i,s}}{\sigma_{i,j}^{(t)}\sigma_{i,s}^{(t)}(1-\rho^{(t)}{}_{i,j,s}^2)}+\frac{Y_{i,j}Y_{i,s}}{\sigma_{i,j}^{(t)}\sigma_{i,s}^{(t)}(1+\rho_{i,j,s}^{(t)})}\Bigg\}\boldsymbol{Z}_i.$$

Next consider,

$$\frac{\partial^2\psi_{1,j,s}(\boldsymbol{\alpha}_j-\boldsymbol{\alpha}_j^{(t)},j|\boldsymbol{\theta}^{(t)})}{\partial\boldsymbol{\alpha}_j\partial\boldsymbol{\alpha}_j^\top}=-\sum_{i=1}^{n}\Bigg[\frac{4Y_{i,j}^2}{\sigma_{i,j}^{(t)^2}(1-\rho_{i,j,s}^{(t)^2})}\exp\{4\boldsymbol{Z}_i^\top(\boldsymbol{\alpha}_j^{(t)}-\boldsymbol{\alpha}_j)\}+\frac{3}{2\sigma_{i,j}^{(t)}\sigma_{i,s}^{(t)}}\left\{\frac{(Y_{i,j}^2+Y_{i,s}^2)}{(1-\rho_{i,j,s}^{(t)^2})}+\frac{(Y_{i,j}+Y_{i,s})^2}{(1+\rho_{i,j,s}^{(t)})}\right\}\exp\{3\boldsymbol{Z}_i^\top(\boldsymbol{\alpha}_j^{(t)}-\boldsymbol{\alpha}_j)\}\Bigg]\boldsymbol{Z}_i\boldsymbol{Z}_i^\top,$$

and

$$\left(\frac{\partial^2\psi_{1,j,s}(\boldsymbol{\alpha}_j-\boldsymbol{\alpha}_j^{(t)},j|\boldsymbol{\theta}^{(t)})}{\partial\boldsymbol{\alpha}_j\partial\boldsymbol{\alpha}_j^\top}\right)_{\boldsymbol{\theta}=\boldsymbol{\theta}^{(t)}}=-\sum_{i=1}^{n}\Bigg[\frac{4Y_{i,j}^2}{\sigma_{i,j}^{(t)^2}(1-\rho_{i,j,s}^{(t)^2})}+\frac{3}{2\sigma_{i,j}^{(t)}\sigma_{i,s}^{(t)}}\left\{\frac{(Y_{i,j}^2+Y_{i,s}^2)}{(1-\rho_{i,j,s}^{(t)^2})}+\frac{(Y_{i,j}+Y_{i,s})^2}{(1+\rho_{i,j,s}^{(t)})}\right\}\Bigg]\boldsymbol{Z}_i\boldsymbol{Z}_i^\top.$$

Similarly,

$$\left(\frac{\partial^2\psi_{1,s,j}(\boldsymbol{\alpha}_j-\boldsymbol{\alpha}_j^{(t)},j|\boldsymbol{\theta}^{(t)})}{\partial\boldsymbol{\alpha}_j\partial\boldsymbol{\alpha}_j^\top}\right)_{\boldsymbol{\theta}=\boldsymbol{\theta}^{(t)}}=-\sum_{i=1}^{n}\Bigg[\frac{4Y_{i,j}^2}{\sigma_{i,j}^{(t)^2}(1-\rho_{i,s,j}^{(t)^2})}+\frac{3}{2\sigma_{i,j}^{(t)}\sigma_{i,s}^{(t)}}\Bigg\{\frac{(Y_{i,j}^2+Y_{i,s}^2)}{(1-\rho_{i,s,j}^{(t)^2})}$$

$$+ \frac{(Y_{i,j} + Y_{i,s})^2}{(1 + \rho_{i,s,j}^{(t)})} \Bigg\} \Bigg] \boldsymbol{Z}_i \boldsymbol{Z}_i^\top.$$

Combining the above two expressions, we obtain

$$\left(\frac{\partial^2 \ell^*(\boldsymbol{\theta}|\boldsymbol{\theta}^{(t)})}{\partial \boldsymbol{\alpha}_j \partial \boldsymbol{\alpha}_j^\top}\right)_{\boldsymbol{\theta}=\boldsymbol{\theta}^{(t)}} = -\sum_{s:s<j}\sum_{i=1}^{n}\left[\frac{4Y_{i,j}^2}{\sigma_{i,j}^{(t)^2}(1-\rho_{i,s,j}^{(t)^2})} + \frac{3}{2\sigma_{i,j}^{(t)}\sigma_{i,s}^{(t)}}\left\{\frac{(Y_{i,j}^2+Y_{i,s}^2)}{(1-\rho_{i,s,j}^{(t)^2})} + \frac{(Y_{i,j}+Y_{i,s})^2}{(1+\rho_{i,s,j}^{(t)})}\right\}\right]\boldsymbol{Z}_i\boldsymbol{Z}_i^\top$$
$$-\sum_{s:s<j}\sum_{i=1}^{n}\left[\frac{4Y_{i,j}^2}{\sigma_{i,j}^{(t)^2}(1-\rho_{i,j,s}^{(t)^2})} + \frac{3}{2\sigma_{i,j}^{(t)}\sigma_{i,s}^{(t)}}\left\{\frac{(Y_{i,j}^2+Y_{i,s}^2)}{(1-\rho_{i,j,s}^{(t)^2})} + \frac{(Y_{i,j}+Y_{i,s})^2}{(1+\rho_{i,j,s}^{(t)})}\right\}\right]\boldsymbol{Z}_i\boldsymbol{Z}_i^\top.$$

Next, observe that $\partial\ell^*(\boldsymbol{\theta}|\boldsymbol{\theta}^{(t)})/\partial\boldsymbol{\delta}_{j,k} = \partial g_2(\boldsymbol{\delta}_{j,k}|\boldsymbol{\theta}^{(t)})/\partial\boldsymbol{\delta}_{j,k} = \partial\psi_{2,j,k}(\boldsymbol{\delta}_{j,k}|\boldsymbol{\theta}^{(t)})/\partial\boldsymbol{\delta}_{j,k}$. Recall that

$$\begin{aligned}
\psi_{2,j,k}(\rho_{j,k}|\boldsymbol{\theta}^{(t)}) &= \sum_{i=1}^{n}\Bigg(-\frac{\log(4)}{2} - 0.5\boldsymbol{\delta}_{j,k}^\top\boldsymbol{Z}_i + \log\{\exp(\boldsymbol{\delta}_{j,k}^\top\boldsymbol{Z}_i)+1\} \\
&\quad - \left(\frac{Y_{i,j}^2}{\sigma_{i,j}^{(t)^2}} + \frac{Y_{i,k}^2}{\sigma_{i,k}^{(t)^2}}\right)\left(1-\rho_{i,j,k}^{(t)^2}\right) \times \frac{\{\exp(\boldsymbol{\delta}_{j,k}^\top\boldsymbol{Z}_i)+1\}^4}{64\exp(2\boldsymbol{\delta}_{j,k}^\top\boldsymbol{Z}_i)} \\
&\quad + \frac{\left(Y_{i,j}+Y_{i,k}\right)^2}{2\sigma_{i,j}^{(t)}\sigma_{i,k}^{(t)}(1-\rho_{i,j,k}^{(t)^2})}\left[\log\left(1-\rho_{i,j,k}^{(t)^2}\right) - \log(4) - \boldsymbol{\delta}_{j,k}^\top\boldsymbol{Z}_i + 2\log\{\exp(\boldsymbol{\delta}_{j,k}^\top\boldsymbol{Z}_i)+1\}\right] \\
&\quad - \frac{\left(Y_{i,j}^2+Y_{i,k}^2\right)}{6\sigma_{i,j}^{(t)}\sigma_{i,k}^{(t)}}\left(1-\rho_{i,j,k}^{(t)^2}\right)^2 \times \frac{\{1+\exp(\boldsymbol{\delta}_{j,k}^\top\boldsymbol{Z}_i)\}^6}{64\exp(3\boldsymbol{\delta}_{j,k}^\top\boldsymbol{Z}_i)} \\
&\quad - \frac{\left(Y_{i,j}+Y_{i,k}\right)^2}{6\sigma_{i,j}^{(t)}\sigma_{i,k}^{(t)}}\left(1+\rho_{i,j,k}^{(t)}\right)^2 \times \frac{\{1+\exp(\boldsymbol{\delta}_{j,k}^\top\boldsymbol{Z}_i)\}^3}{8\exp(3\boldsymbol{\delta}_{j,k}^\top\boldsymbol{Z}_i)} \\
&\quad + \frac{\left(Y_{i,j}^2+Y_{i,k}^2\right)}{2\sigma_{i,j}^{(t)}\sigma_{i,k}^{(t)}(1+\rho_{i,j,k}^{(t)})}\left[\log\left(1+\rho_{i,j,k}^{(t)}\right) - \log(2) - \boldsymbol{\delta}_{j,k}^\top\boldsymbol{Z}_i + \log\{1+\exp(\boldsymbol{\delta}_{j,k}^\top\boldsymbol{Z}_i)\}\right]\Bigg) \\
&= \sum_{i=1}^{n}\Bigg(-\frac{\log(4)}{2} - 0.5\boldsymbol{\delta}_{j,k}^\top\boldsymbol{Z}_i + \log\{\exp(\boldsymbol{\delta}_{j,k}^\top\boldsymbol{Z}_i)+1\} \\
&\quad - \left(\frac{Y_{i,j}^2}{\sigma_{i,j}^{(t)^2}} + \frac{Y_{i,k}^2}{\sigma_{i,k}^{(t)^2}}\right)\left(1-\rho_{i,j,k}^{(t)^2}\right) \times \frac{1}{64}\left\{\exp(\boldsymbol{\delta}_{j,k}^\top\boldsymbol{Z}_i/2) + \exp(-\boldsymbol{\delta}_{j,k}^\top\boldsymbol{Z}_i/2)\right\}^4 \\
&\quad + \frac{\left(Y_{i,j}+Y_{i,k}\right)^2}{2\sigma_{i,j}^{(t)}\sigma_{i,k}^{(t)}(1-\rho_{i,j,k}^{(t)^2})}\left[\log\left(1-\rho_{i,j,k}^{(t)^2}\right) - \log(4) - \boldsymbol{\delta}_{j,k}^\top\boldsymbol{Z}_i + 2\log\{\exp(\boldsymbol{\delta}_{j,k}^\top\boldsymbol{Z}_i)+1\}\right] \\
&\quad - \frac{\left(Y_{i,j}^2+Y_{i,k}^2\right)}{6\sigma_{i,j}^{(t)}\sigma_{i,k}^{(t)}}\left(1-\rho_{i,j,k}^{(t)}\right)^2 \times \frac{1}{64}\left\{\exp(\boldsymbol{\delta}_{j,k}^T\boldsymbol{Z}_i/2) + \exp(-\boldsymbol{\delta}_{j,k}^\top\boldsymbol{Z}_i/2)\right\}^6
\end{aligned}$$

$$
- \frac{\left(Y_{i,j} + Y_{i,k}\right)^2}{6\sigma_{i,j}^{(t)}\sigma_{i,k}^{(t)}} \left(1+\rho_{i,j,k}^{(t)}\right)^2 \times \frac{1}{8}\left\{1+\exp(-\boldsymbol{\delta}_{j,k}^\top \boldsymbol{Z}_i)\right\}^3
$$

$$
+ \frac{\left(Y_{i,j}^2 + Y_{i,k}^2\right)}{2\sigma_{i,j}^{(t)}\sigma_{i,k}^{(t)}(1+\rho_{i,j,k}^{(t)})}\left[\log\left(1+\rho_{i,j,k}^{(0)}\right) - \log(2) - \boldsymbol{\delta}_{j,k}^\top \boldsymbol{Z}_i + \log\{1+\exp(\boldsymbol{\delta}_{j,k}^\top \boldsymbol{Z}_i)\}\right]\Bigg).
$$

Now,

$$
\begin{aligned}
&\frac{\partial \psi_{2,j,k}(\rho_{j,k}|\boldsymbol{\theta}^{(t)})}{\partial \boldsymbol{\delta}_{j,k}} \\
&= \sum_{i=1}^n \Bigg[-0.5 + \frac{\exp(\boldsymbol{\delta}_{j,k}^\top \boldsymbol{Z}_i)}{1+\exp(\boldsymbol{\delta}_{j,k}^\top \boldsymbol{Z}_i)} \\
&- \left(\frac{Y_{i,j}^2}{\sigma_{i,j}^{(t)^2}} + \frac{Y_{i,k}^2}{\sigma_{i,k}^{(t)^2}}\right)\left(1-\rho_{i,j,k}^{(t)^2}\right) \times \frac{1}{32}\left\{\exp(\boldsymbol{\delta}_{j,k}^\top \boldsymbol{Z}_i/2) + \exp(-\boldsymbol{\delta}_{j,k}^\top \boldsymbol{Z}_i/2)\right\}^3 \\
&\times \left\{\exp(\boldsymbol{\delta}_{j,k}^\top \boldsymbol{Z}_i/2) - \exp(-\boldsymbol{\delta}_{j,k}^\top \boldsymbol{Z}_i/2)\right\} \\
&+ \frac{\left(Y_{i,j} + Y_{i,k}\right)^2}{2\sigma_{i,j}^{(t)}\sigma_{i,k}^{(t)}(1-\rho_{i,j,k}^{(t)^2})}\left\{-1 + \frac{2\exp(\boldsymbol{\delta}_{j,k}^\top \boldsymbol{Z}_i)}{1+\exp(\boldsymbol{\delta}_{j,k}^\top \boldsymbol{Z}_i)}\right\} \\
&- \frac{\left(Y_{i,j}^2 + Y_{i,k}^2\right)}{6\sigma_{i,j}^{(t)}\sigma_{i,k}^{(t)}}\left(1-\rho_{i,j,k}^{(t)^2}\right)^2 \times \frac{3}{64}\left\{\exp(\boldsymbol{\delta}_{j,k}^\top \boldsymbol{Z}_i/2) + \exp(-\boldsymbol{\delta}_{j,k}^\top \boldsymbol{Z}_i/2)\right\}^5 \\
&\times \left\{\exp(\boldsymbol{\delta}_{j,k}^\top \boldsymbol{Z}_i/2) - \exp(-\boldsymbol{\delta}_{j,k}^\top \boldsymbol{Z}_i/2)\right\} \\
&- \frac{\left(Y_{i,j} + Y_{i,k}\right)^2}{6\sigma_{i,j}^{(t)}\sigma_{i,k}^{(t)}}\left(1+\rho_{i,j,k}^{(t)}\right)^2 \times \frac{3}{8}\left\{1+\exp(-\boldsymbol{\delta}_{j,k}^\top \boldsymbol{Z}_i)\right\}^2\left\{1-\exp(-\boldsymbol{\delta}_{j,k}^\top \boldsymbol{Z}_i)\right\} \\
&+ \frac{\left(Y_{i,j}^2 + Y_{i,k}^2\right)}{2\sigma_{i,j}^{(t)}\sigma_{i,k}^{(t)}(1+\rho_{i,j,k}^{(t)})}\left\{-1 + \frac{\exp(\boldsymbol{\delta}_{j,k}^\top \boldsymbol{Z}_i)}{1+\exp(\boldsymbol{\delta}_{j,k}^\top \boldsymbol{Z}_i)}\right\}\Bigg]\boldsymbol{Z}_i,
\end{aligned}
$$

and

$$
\begin{aligned}
\left(\frac{\partial \psi_{2,j,k}(\rho_{j,k}|\boldsymbol{\theta}^{(t)})}{\partial \boldsymbol{\delta}_{j,k}}\right)_{\boldsymbol{\theta}=\boldsymbol{\theta}^{(t)}} &= \sum_{i=1}^n \Bigg[-0.5 + \frac{\exp(\boldsymbol{Z}_i^\top \boldsymbol{\delta}_{j,k}^{(t)})}{1+\exp(\boldsymbol{Z}_i^\top \boldsymbol{\delta}_{j,k}^{(t)})} \\
&- \left(\frac{Y_{i,j}^2}{\sigma_{i,j}^{(t)^2}} + \frac{Y_{i,k}^2}{\sigma_{i,k}^{(t)^2}}\right)\left(1-\rho_{i,j,k}^{(t)^2}\right) \times \frac{1}{32}\left\{\exp(\boldsymbol{Z}_i^\top \boldsymbol{\delta}_{j,k}^{(t)}/2) + \exp(-\boldsymbol{Z}_i^\top \boldsymbol{\delta}_{j,k}^{(t)}/2)\right\}^3
\end{aligned}
$$

$$\times \left\{\exp(\boldsymbol{Z}_i^\top \boldsymbol{\delta}_{j,k}^{(t)}/2) - \exp(-\boldsymbol{Z}_i^\top \boldsymbol{\delta}_{j,k}^{(t)}/2)\right\}$$

$$+ \frac{\left(Y_{i,j} + Y_{i,k}\right)^2}{2\sigma_{i,j}^{(t)}\sigma_{i,k}^{(t)}(1-\rho_{i,j,k}^{(t)^2})} \left\{-1 + \frac{2\exp(\boldsymbol{Z}_i^\top \boldsymbol{\delta}_{j,k}^{(t)})}{1+\exp(\boldsymbol{Z}_i^\top \boldsymbol{\delta}_{j,k}^{(t)})}\right\}$$

$$- \frac{\left(Y_{i,j}^2 + Y_{i,k}^2\right)}{6\sigma_{i,j}^{(t)}\sigma_{i,k}^{(t)}} \left(1-\rho_{i,j,k}^{(t)^2}\right)^2 \times \frac{3}{64}\left\{\exp(\boldsymbol{Z}_i^\top \boldsymbol{\delta}_{j,k}^{(t)}/2) + \exp(-\boldsymbol{Z}_i^\top \boldsymbol{\delta}_{j,k}^{(t)}/2)\right\}^5$$

$$\times \left\{\exp(\boldsymbol{Z}_i^\top \boldsymbol{\delta}_{j,k}^{(t)}/2) - \exp(-\boldsymbol{Z}_i^\top \boldsymbol{\delta}_{j,k}^{(t)}/2)\right\}$$

$$- \frac{\left(Y_{i,j} + Y_{i,k}\right)^2}{6\sigma_{i,j}^{(t)}\sigma_{i,k}^{(t)}} \left(1+\rho_{i,j,k}^{(t)}\right)^2 \times \frac{3}{8}\left\{1 + \exp(-\boldsymbol{Z}_i^\top \boldsymbol{\delta}_{j,k}^{(t)})\right\}^2 \left\{1 - \exp(-\boldsymbol{Z}_i^\top \boldsymbol{\delta}_{j,k}^{(t)})\right\}$$

$$+ \frac{\left(Y_{i,j}^2 + Y_{i,k}^2\right)}{2\sigma_{i,j}^{(t)}\sigma_{i,k}^{(t)}(1+\rho_{i,j,k}^{(t)})}\left\{-1 + \frac{\exp(\boldsymbol{Z}_i^\top \boldsymbol{\delta}_{j,k}^{(t)})}{1+\exp(\boldsymbol{Z}_i^\top \boldsymbol{\delta}_{j,k}^{(t)})}\right\}\Bigg] \boldsymbol{Z}_i.$$

Simplifying further, we obtain

$$\left(\frac{\partial \ell^*(\boldsymbol{\theta}|\boldsymbol{\theta}^{(t)})}{\partial \boldsymbol{\delta}_{j,k}}\right)_{\boldsymbol{\theta}=\boldsymbol{\theta}^{(t)}} = \sum_{i=1}^n \left\{ \frac{\rho_{i,j,k}^{(t)}}{1-\rho_{i,j,k}^{(t)^2}} - \frac{Y_{i,j}^2 \rho_{i,j,k}^{(t)}}{{\sigma^{(t)}}_{i,j}^2(1-\rho_{i,j,k}^{(t)^2})^2} - \frac{Y_{i,k}^2 \rho_{i,j,k}^{(t)}}{{\sigma^{(t)}}_{i,k}^2(1-\rho_{i,j,k}^{(t)^2})^2} \right.$$
$$\left. + \frac{2Y_{i,j}Y_{i,k}\rho_{i,j,k}^{(t)}}{\sigma_{i,j}^{(t)}\sigma_{i,k}^{(t)}(1-\rho_{i,j,k}^{(t)^2})^2} + \frac{Y_{i,j}Y_{i,k}}{\sigma_{i,j}^{(t)}\sigma_{i,k}^{(t)}(1+\rho_{i,j,k}^{(t)})^2}\right\} \frac{(1-\rho_{i,j,k}^{(t)^2})}{2} \boldsymbol{Z}_i.$$

Next,

$$\frac{\partial^2 \psi_{2,j,k}(\rho_{j,k}|\boldsymbol{\theta}^{(t)})}{\partial \boldsymbol{\delta}_{j,k}\partial \boldsymbol{\delta}_{j,k}^\top} = \sum_{i=1}^n \Bigg(\frac{\exp(\boldsymbol{\delta}_{j,k}^T \boldsymbol{Z}_i)}{\{1+\exp(\boldsymbol{\delta}_{j,k}^\top \boldsymbol{Z}_i)\}^2}$$

$$- \left(\frac{Y_{i,j}^2}{\sigma_{i,j}^{(t)^2}} + \frac{Y_{i,k}^2}{\sigma_{i,k}^{(t)^2}}\right)\left(1-\rho_{i,j,k}^{(t)^2}\right) \times \frac{1}{64}\Big[3\{\exp(\boldsymbol{\delta}_{j,k}^\top \boldsymbol{Z}_i/2) + \exp(-\boldsymbol{\delta}_{j,k}^\top \boldsymbol{Z}_i/2)\}^2$$

$$\times \{\exp(\boldsymbol{\delta}_{j,k}^\top \boldsymbol{Z}_i/2) - \exp(-\boldsymbol{\delta}_{j,k}^\top \boldsymbol{Z}_i/2)\}^2 + \{\exp(\boldsymbol{\delta}_{j,k}^\top \boldsymbol{Z}_i/2) + \exp(-\boldsymbol{\delta}_{j,k}^\top \boldsymbol{Z}_i/2)\}^4\Big]$$

$$+ \frac{\left(Y_{i,j} + Y_{i,k}\right)^2}{2\sigma_{i,j}^{(t)}\sigma_{i,k}^{(t)}(1-\rho_{i,j,k}^{(t)^2})} \times \frac{2\exp(\boldsymbol{\delta}_{j,k}^\top \boldsymbol{Z}_i)}{\{1+\exp(\boldsymbol{\delta}_{j,k}^\top \boldsymbol{Z}_i)\}^2}$$

$$- \frac{\left(Y_{i,j}^2 + Y_{i,k}^2\right)}{6\sigma_{i,j}^{(t)}\sigma_{i,k}^{(t)}} \left(1-\rho_{i,j,k}^{(t)^2}\right)^2 \times \frac{3}{128}\Big[5\{\exp(\boldsymbol{\delta}_{j,k}^\top \boldsymbol{Z}_i/2) + \exp(-\boldsymbol{\delta}_{j,k}^\top \boldsymbol{Z}_i/2)\}^4$$

$$\times \{\exp(\boldsymbol{\delta}_{j,k}^\top \boldsymbol{Z}_i/2) - \exp(-\boldsymbol{\delta}_{j,k}^\top \boldsymbol{Z}_i/2)\}^2 + \{\exp(\boldsymbol{\delta}_{j,k}^\top \boldsymbol{Z}_i/2) + \exp(-\boldsymbol{\delta}_{j,k}^\top \boldsymbol{Z}_i/2)\}^6\Big]$$

$$- \frac{\left(Y_{i,j} + Y_{i,k}\right)^2}{6\sigma_{i,j}^{(t)}\sigma_{i,k}^{(t)}} \left(1 + \rho_{i,j,k}^{(t)}\right)^2 \times \frac{3}{8}\Big[2\{1 + \exp(-\boldsymbol{\delta}_{j,k}^\top \boldsymbol{Z}_i)\}\{1 - \exp(-\boldsymbol{\delta}_{j,k}^\top \boldsymbol{Z}_i)\}^2$$

$$+ \{\exp(\boldsymbol{\delta}_{j,k}^\top \boldsymbol{Z}_i) + \exp(-\boldsymbol{\delta}_{j,k}^\top \boldsymbol{Z}_i)\}^3\Big] + \frac{\left(Y_{i,j}^2 + Y_{i,k}^2\right)}{2\sigma_{i,j}^{(t)}\sigma_{i,k}^{(t)}(1 + \rho_{i,j,k}^{(t)})} \times \frac{\exp(\boldsymbol{\delta}_{j,k}^\top \boldsymbol{Z}_i)}{\{1 + \exp(\boldsymbol{\delta}_{j,k}^\top \boldsymbol{Z}_i)\}^2}\Bigg) \boldsymbol{Z}_i \boldsymbol{Z}_i^\top.$$

Subsequently,

$$\left(\frac{\partial^2 \psi_{2,j,k}(\rho_{j,k}|\boldsymbol{\theta}^{(t)})}{\partial \boldsymbol{\delta}_{j,k} \partial \boldsymbol{\delta}_{j,k}^\top}\right)_{\boldsymbol{\theta}=\boldsymbol{\theta}^{(t)}} = \sum_{i=1}^{n} \Bigg(\frac{\exp(\boldsymbol{Z}_i^\top \boldsymbol{\delta}_{j,k}^{(t)})}{\{1 + \exp(\boldsymbol{Z}_i^\top \boldsymbol{\delta}_{j,k}^{(t)})\}^2}$$

$$- \left(\frac{Y_{i,j}^2}{\sigma_{i,j}^{(t)^2}} + \frac{Y_{i,k}^2}{\sigma_{i,k}^{(t)^2}}\right) \left(1 - \rho_{i,j,k}^{(t)^2}\right) \times \frac{1}{64}\Big[3\{\exp(\boldsymbol{Z}_i^\top \boldsymbol{\delta}_{j,k}^{(t)}/2) + \exp(-\boldsymbol{Z}_i^\top \boldsymbol{\delta}_{j,k}^{(t)}/2)\}^2$$

$$\times \{\exp(\boldsymbol{Z}_i^\top \boldsymbol{\delta}_{j,k}^{(t)}/2) - \exp(-\boldsymbol{Z}_i^\top \boldsymbol{\delta}_{j,k}^{(t)}/2)\}^2$$

$$+ \{\exp(\boldsymbol{Z}_i^\top \boldsymbol{\delta}_{j,k}^{(t)}/2) + \exp(-\boldsymbol{Z}_i^\top \boldsymbol{\delta}_{j,k}^{(t)}/2)\}^4\Big]$$

$$+ \frac{\left(Y_{i,j} + Y_{i,k}\right)^2}{2\sigma_{i,j}^{(t)}\sigma_{i,k}^{(t)}(1 - \rho_{i,j,k}^{(t)^2})} \times \frac{2\exp(\boldsymbol{Z}_i^\top \boldsymbol{\delta}_{j,k}^{(t)})}{\{1 + \exp(\boldsymbol{Z}_i^\top \boldsymbol{\delta}_{j,k}^{(t)})\}^2}$$

$$- \frac{\left(Y_{i,j}^2 + Y_{i,k}^2\right)}{6\sigma_{i,j}^{(t)}\sigma_{i,k}^{(t)}} \left(1 - \rho_{i,j,k}^{(t)^2}\right)^2 \times \frac{3}{128}\Big[5\{\exp(\boldsymbol{Z}_i^\top \boldsymbol{\delta}_{j,k}^{(t)}/2) + \exp(-\boldsymbol{Z}_i^\top \boldsymbol{\delta}_{j,k}^{(t)}/2)\}^4$$

$$\times \{\exp(\boldsymbol{Z}_i^\top \boldsymbol{\delta}_{j,k}^{(t)}/2) - \exp(-\boldsymbol{Z}_i^\top \boldsymbol{\delta}_{j,k}^{(t)}/2)\}^2$$

$$+ \{\exp(\boldsymbol{Z}_i^\top \boldsymbol{\delta}_{j,k}^{(t)}/2) + \exp(-\boldsymbol{Z}_i^\top \boldsymbol{\delta}_{j,k}^{(t)}/2)\}^6\Big]$$

$$- \frac{\left(Y_{i,j} + Y_{i,k}\right)^2}{6\sigma_{i,j}^{(t)}\sigma_{i,k}^{(t)}} \left(1 + \rho_{i,j,k}^{(t)}\right)^2 \times \frac{3}{8}\Big[2\{1 + \exp(-\boldsymbol{Z}_i^\top \boldsymbol{\delta}_{j,k}^{(t)})\}\{1 - \exp(-\boldsymbol{Z}_i^\top \boldsymbol{\delta}_{j,k}^{(t)})\}^2$$

$$+ \{\exp(\boldsymbol{Z}_i^\top \boldsymbol{\delta}_{j,k}^{(t)}) + \exp(-\boldsymbol{Z}_i^\top \boldsymbol{\delta}_{j,k}^{(t)})\}^3\Big] + \frac{\left(Y_{i,j}^2 + Y_{i,k}^2\right)}{2\sigma_{i,j}^{(t)}\sigma_{i,k}^{(t)}(1 + \rho_{i,j,k}^{(t)})}$$

$$\times \frac{\exp(\boldsymbol{Z}_i^\top \boldsymbol{\delta}_{j,k}^{(t)})}{\{1 + \exp(\boldsymbol{Z}_i^\top \boldsymbol{\delta}_{j,k}^{(t)})\}^2}\Bigg) \boldsymbol{Z}_i \boldsymbol{Z}_i^\top.$$

Simplifying further, we obtain,

$$
\begin{aligned}
\left(\frac{\partial^2 \ell^*(\boldsymbol{\theta}|\boldsymbol{\theta}^{(t)})}{\partial \boldsymbol{\delta}_{j,k} \partial \boldsymbol{\delta}_{j,k}^\top}\right)_{\boldsymbol{\theta}=\boldsymbol{\theta}^{(t)}} &= \sum_{i=1}^n \Bigg[\frac{1+\rho_{i,j,k}^{(t)^2}}{(1-\rho_{i,j,k}^{(t)^2})^2} - \left(\frac{Y_{i,j}^2}{\sigma_{i,j}^{(t)^2}} + \frac{Y_{i,k}^2}{\sigma_{i,k}^{(t)^2}}\right) \times \frac{1+5\rho_{i,j,k}^{(t)^2}}{(1-\rho_{i,j,k}^{(t)^2})^3} \\
&+ \frac{1}{\sigma_{i,j}^{(t)}\sigma_{i,k}^{(t)}(1-\rho_{i,j,k}^{(t)^2})^3}\left\{(Y_{i,j}+Y_{i,k})^2(1+\rho_{i,j,k}^{(t)^2}) - (Y_{i,j}^2+Y_{i,k}^2)(1+7\rho_{i,j,k}^{(t)^2})\right\} \\
&+ \frac{Y_{i,j}^2+Y_{i,k}^2-4(Y_{i,j}+Y_{i,k})^2}{2\sigma_{i,j}^{(t)}\sigma_{i,k}^{(t)}(1+\rho_{i,j,k}^{(t)})^3}\Bigg] \frac{(1-\rho_{i,j,k}^{(t)^2})^2}{4} \boldsymbol{Z}_i \boldsymbol{Z}_i^\top \\
&+ \sum_{i=1}^n \Bigg[\frac{\rho_{i,j,k}^{(t)}}{1-\rho_{i,j,k}^{(t)^2}} - \left(\frac{Y_{i,j}^2}{{\sigma^{(t)}}_{i,j}^2} + \frac{Y_{i,k}^2}{{\sigma^{(t)}}_{i,k}^2}\right) \frac{\rho_{i,j,k}^{(t)}}{(1-\rho_{i,j,k}^{(t)^2})^2} \\
&- \frac{Y_{i,j}Y_{i,k}}{\sigma_{i,j}^{(t)}\sigma_{i,k}^{(t)}}\left\{\frac{2\rho_{i,j,k}^{(t)}}{(1-\rho_{i,j,k}^{(t)^2})^2} + \frac{1}{(1+\rho_{i,j,k}^{(t)})^2}\right\}\Bigg] \frac{\rho_{i,j,k}^{(t)}(1-\rho_{i,j,k}^{(t)^2})}{2} \boldsymbol{Z}_i \boldsymbol{Z}_i^\top .
\end{aligned}
$$

A.4 Detailed expressions of the terms in Section 4

Let $\ell_{i,j,k}(\boldsymbol{\alpha},\boldsymbol{\delta}) = \log\{f(Y_{i,j}, Y_{i,k}|\boldsymbol{X}_i)\}$, and $\ell_i(\boldsymbol{\alpha},\boldsymbol{\delta}) = \sum_j \sum_{j<k} \log\{f(Y_{i,j}, Y_{i,k}|\boldsymbol{X}_i)\}$. Then,

$$
\ell_{i,j,k}(\boldsymbol{\alpha},\boldsymbol{\delta}) = -\frac{1}{2}\left[\log(\sigma_{i,j}^2) + \log(\sigma_{i,k}^2) + \log(1-\rho_{i,j,k}^2) + \frac{1}{(1-\rho_{i,j,k}^2)}\left(\frac{Y_{i,j}^2}{\sigma_{i,j}^2} - \frac{2\rho_{i,j,k}Y_{i,j}Y_{i,k}}{\sigma_{i,j}\sigma_{i,k}} + \frac{Y_{i,k}^2}{\sigma_{i,k}^2}\right)\right]
$$

and

$$
\begin{aligned}
\ell_i(\boldsymbol{\alpha},\boldsymbol{\delta}) &= -\frac{1}{2}\sum_{j=1}^{q-1}\sum_{k=j+1}^{q}\left[\log(\sigma_{i,j}^2) + \log(\sigma_{i,k}^2) + \log(1-\rho_{i,j,k}^2) + \frac{1}{(1-\rho_{i,j,k}^2)}\left(\frac{Y_{i,j}^2}{\sigma_{i,j}^2} - \frac{2\rho_{i,j,k}Y_{i,j}Y_{i,k}}{\sigma_{i,j}\sigma_{i,k}} + \frac{Y_{i,k}^2}{\sigma_{i,k}^2}\right)\right] \\
&= -\frac{1}{2}\sum_{j=1}^{q}(q-1)\log(\sigma_{i,j}^2) - \frac{1}{2}\sum_{j<k}\sum \log(1-\rho_{i,j,k}^2) \\
&\quad - \frac{1}{2}\sum_{j<k}\sum \frac{1}{(1-\rho_{i,j,k}^2)}\left(\frac{Y_{i,j}^2}{\sigma_{i,j}^2} - \frac{2\rho_{i,j,k}Y_{i,j}Y_{i,k}}{\sigma_{i,j}\sigma_{i,k}} + \frac{Y_{i,k}^2}{\sigma_{i,k}^2}\right).
\end{aligned}
$$

We need to calculate the score functions $\mathcal{U}(\boldsymbol{\theta}; D_i) = \partial \ell_i(\boldsymbol{\alpha},\boldsymbol{\delta})/\partial\boldsymbol{\theta}$. For this derivation we use $\partial\sigma_{i,j}/\partial\boldsymbol{\alpha}_j = \sigma_{i,j}\boldsymbol{Z}_i$ and $\partial\rho_{i,j,k}/\partial\boldsymbol{\delta}_{j,k} = 0.5(1-\rho_{i,j,k}^2)\boldsymbol{Z}_i$. For $j = 1, \ldots, q$,

$$
\begin{aligned}
\frac{\partial \ell_i(\boldsymbol{\alpha},\boldsymbol{\delta})}{\partial \boldsymbol{\alpha}_j} &= -\frac{(q-1)}{\sigma_{i,j}}\frac{\partial\sigma_{i,j}}{\partial\boldsymbol{\alpha}_j} + \sum_{k=1,k\neq j}^{q} \frac{Y_{i,j}^2}{(1-\rho_{i,j,k}^2)\sigma_{i,j}^3}\frac{\partial\sigma_{i,j}}{\partial\boldsymbol{\alpha}_j} - \sum_{k=1,k\neq j}^{q} \frac{\rho_{i,j,k}Y_{i,j}Y_{i,k}}{(1-\rho_{i,j,k}^2)\sigma_{i,k}\sigma_{i,j}^2}\frac{\partial\sigma_{i,j}}{\partial\boldsymbol{\alpha}_j} \\
&= -(q-1)\boldsymbol{Z}_i + \sum_{k=1,k\neq j}^{q} \frac{Y_{i,j}^2}{(1-\rho_{i,j,k}^2)\sigma_{i,j}^2}\boldsymbol{Z}_i - \sum_{k=1,k\neq j}^{q} \frac{\rho_{i,j,k}Y_{i,j}Y_{i,k}}{(1-\rho_{i,j,k}^2)\sigma_{i,k}\sigma_{i,j}}\boldsymbol{Z}_i,
\end{aligned}
$$

$$
\begin{aligned}
\frac{\partial \ell_i(\boldsymbol{\alpha},\boldsymbol{\delta})}{\partial \boldsymbol{\delta}_{j,k}} &= \frac{\rho_{i,j,k}}{(1-\rho_{i,j,k}^2)}\frac{\partial \rho_{i,j,k}}{\partial \boldsymbol{\delta}_{j,k}} - \left(\frac{Y_{i,j}^2}{\sigma_{i,j}^2}+\frac{Y_{i,k}^2}{\sigma_{i,k}^2}\right)\frac{\rho_{i,j,k}}{(1-\rho_{i,j,k}^2)^2}\frac{\partial \rho_{i,j,k}}{\partial \boldsymbol{\delta}_{j,k}} \\
&\quad + \frac{Y_{i,j}Y_{i,k}}{\sigma_{i,j}\sigma_{i,k}}\left((1-\rho_{i,j,k}^2)^{-1}\frac{\partial \rho_{i,j,k}}{\partial \boldsymbol{\delta}_{j,k}} + \frac{2\rho_{i,j,k}^2}{(1-\rho_{i,j,k}^2)^2}\frac{\partial \rho_{i,j,k}}{\partial \boldsymbol{\delta}_{j,k}}\right) \\
&= \frac{\rho_{i,j,k}}{2}\boldsymbol{Z}_i - \frac{1}{2}\left(\frac{Y_{i,j}^2}{\sigma_{i,j}^2}+\frac{Y_{i,k}^2}{\sigma_{i,k}^2}\right)\frac{\rho_{i,j,k}}{(1-\rho_{i,j,k}^2)}\boldsymbol{Z}_i + \frac{Y_{i,j}Y_{i,k}}{\sigma_{i,j}\sigma_{i,k}}\left(\frac{\boldsymbol{Z}_i}{2} + \frac{\rho_{i,j,k}^2}{(1-\rho_{i,j,k}^2)}\boldsymbol{Z}_i\right),
\end{aligned}
$$

for $j<k$. To calculate the sensitivity matrix, we need to calculate the double derivatives of the above two expressions. That is for $j=1,\ldots,q$

$$
\begin{aligned}
\frac{\partial^2 \ell_i(\boldsymbol{\alpha},\boldsymbol{\delta})}{\partial \boldsymbol{\alpha}_j \partial \boldsymbol{\alpha}_j^\top} &= \sum_{k=1,k\neq j}^{q} -2\left(\frac{Y_{i,j}^2}{(1-\rho_{i,j,k}^2)\sigma_{i,j}^3}\right)\boldsymbol{Z}_i\frac{\partial \sigma_{i,j}}{\partial \boldsymbol{\alpha}_j^\top} + \sum_{k=1,k\neq j}^{q}\left(\frac{\rho_{i,j,k}Y_{i,j}Y_{i,k}}{\sigma_{i,j}^2\sigma_{i,k}}\right)\boldsymbol{Z}_i\frac{\partial \sigma_{i,j}}{\partial \boldsymbol{\alpha}_j^\top} \\
&= -2\sum_{k=1,k\neq j}^{q}\left(\frac{Y_{i,j}^2}{(1-\rho_{i,j,k}^2)\sigma_{i,j}^2}\right)\boldsymbol{Z}_i\boldsymbol{Z}_i^\top + \sum_{k=1,k\neq j}^{q}\left(\frac{\rho_{i,j,k}Y_{i,j}Y_{i,k}}{\sigma_{i,j}\sigma_{i,k}}\right)\boldsymbol{Z}_i\boldsymbol{Z}_i^\top, \\
\frac{\partial^2 \ell_i(\boldsymbol{\alpha},\boldsymbol{\delta})}{\partial \boldsymbol{\alpha}_j \partial \boldsymbol{\alpha}_k^\top} &= \frac{\rho_{i,j,k}Y_{i,j}Y_{i,k}}{(1-\rho_{i,j,k}^2)\sigma_{i,j}\sigma_{i,k}}\boldsymbol{Z}_i\boldsymbol{Z}_i^\top,
\end{aligned}
$$

and for $j<k$

$$
\begin{aligned}
\frac{\partial^2 \ell_i(\boldsymbol{\alpha},\boldsymbol{\delta})}{\partial \boldsymbol{\alpha}_j \partial \boldsymbol{\delta}_{j,k}^\top} &= \left\{\frac{Y_{i,j}^2\rho_{i,j,k}}{\sigma_{i,j}^2(1-\rho_{i,j,k}^2)} - \frac{Y_{i,j}Y_{i,k}}{\sigma_{i,j}\sigma_{i,k}}\left(\frac{1}{2}+\frac{\rho_{i,j,k}^2}{1-\rho_{i,j,k}^2}\right)\right\}\boldsymbol{Z}_i\boldsymbol{Z}_i^\top, \\
\frac{\partial^2 \ell_i(\boldsymbol{\alpha},\boldsymbol{\delta})}{\partial \boldsymbol{\delta}_{j,k} \partial \boldsymbol{\delta}_{j,k}^\top} &= \frac{(1-\rho_{i,j,k}^2)\boldsymbol{Z}_i\boldsymbol{Z}_i^\top}{4} - \frac{\boldsymbol{Z}_i}{2}\left(\frac{Y_{i,j}^2}{\sigma_{i,j}^2}+\frac{Y_{i,k}^2}{\sigma_{i,k}^2}\right)\left((1-\rho_{i,j,k}^2)^{-1}\frac{\partial \rho_{i,j,k}}{\partial \boldsymbol{\delta}_{j,k}^\top} + \frac{2\rho_{i,j,k}^2}{(1-\rho_{i,j,k}^2)^2}\frac{\partial \rho_{i,j,k}}{\partial \boldsymbol{\delta}_{j,k}^\top}\right) \\
&\quad + \frac{Y_{i,j}Y_{i,k}\boldsymbol{Z}_i}{\sigma_{i,j}\sigma_{i,k}}\left(\frac{2\rho_{i,j,k}^3}{(1-\rho_{i,j,k}^2)^2}\frac{\partial \rho_{i,j,k}}{\partial \boldsymbol{\delta}_{j,k}^\top} + \frac{2\rho_{i,j,k}}{(1-\rho_{i,j,k}^2)}\frac{\partial \rho_{i,j,k}}{\partial \boldsymbol{\delta}_{j,k}^\top}\right) \\
&= \left\{\frac{(1-\rho_{i,j,k}^2)}{4} - \frac{1}{2}\left(\frac{Y_{i,j}^2}{\sigma_{i,j}^2}+\frac{Y_{i,k}^2}{\sigma_{i,k}^2}\right)\left(\frac{1}{2}+\frac{\rho_{i,j,k}^2}{(1-\rho_{i,j,k}^2)}\right)\right. \\
&\quad \left. + \frac{Y_{i,j}Y_{i,k}}{\sigma_{i,j}\sigma_{i,k}}\left(\frac{\rho_{i,j,k}^3}{(1-\rho_{i,j,k}^2)} + \rho_{i,j,k}\right)\right\}\boldsymbol{Z}_i\boldsymbol{Z}_i^\top.
\end{aligned}
$$

A.5 Computational advantage

We have extended Scenario 3 from the simulation design in the manuscript by varying the number of predictor variables. Specifically, we set the number of phenotypes, q to 4, and the sample size, n to 500. We used four different values of the predictor variable, p= $2,3,4,5$. This resulted in the number of unknown parameters in our setting as

$30, 40, 50, 60$ respectively. The multivariate phenotype response, Y, and the design matrix, X were generated exactly as in Section 5 of the manuscript. Under each scenario, we performed 100 simulations. Figure 4 shows the average computation time (in seconds) of the MM algorithm and direct optimization (DOP) via the optim function with the "L-BFGS-B" method. Both techniques were used to maximize the pairwise composite likelihood function. The numerical results seem to indicate that the DOP method has an exponential time complexity, and our proposed MM has linear time complexity with respect to the number of parameters.

A.6 Marginal effect estimation

We can use the correlation model to compute another interpretable measure, such as the average marginal effect (AME) (Leeper, 2021; Hugues, 2016; Greene, 1997). In general, AME on the mean is defined as the change in the conditional mean of an outcome variable with respect to a single feature. Likewise, the AME of the rth feature on the (j,k)th pairwise correlation can be defined as the average change of the correlation for a change in the rth feature. Let us denote the $(p-1)$ component vector $(X_{i,1},\ldots,X_{i,r-1},X_{i,r+1},\ldots,X_{i,p})^\top$ by $\boldsymbol{X}_{i,(-r)}$. Then, for a binary feature $\boldsymbol{X}_r$, the AME is defined as $AME_r = E\{\rho_{i,j,k}|X_{i,r} = 1, \boldsymbol{X}_{i,(-r)}\} - E\{\rho_{i,j,k}|X_{i,r} = 0, \boldsymbol{X}_{i,(-r)}\} = E\{\varphi_{r,(j,k)}(\boldsymbol{X}_i,\boldsymbol{\theta})\}$, where $\boldsymbol{\theta}$ denotes all the parameters and $\varphi_{r,(j,k)}(\boldsymbol{X}_i,\boldsymbol{\theta}) = 2[\{1+\exp(\delta_{j,k,0}+\sum_{s\neq r}^{p}\delta_{j,k,s}X_{i,s})\}^{-1} - \{1+\exp(\delta_{j,k,0}+\delta_{j,k,r}+\sum_{s\neq r}^{p}\delta_{j,k,s}X_{i,s})\}^{-1}]$. For a continuous feature $\boldsymbol{X}_r$, $AME_r = E\{\varphi_{r,(j,k)}(\boldsymbol{X}_i,\boldsymbol{\theta})\}$, where $\varphi_{r,(j,k)}(\boldsymbol{X}_i,\boldsymbol{\theta}) = (\partial\rho_{i,j,k}/\partial X_{i,r}) = 2\delta_{j,k,r}\exp(\delta_{j,k,0}+\sum_{s=1}^{p}\delta_{j,k,s}X_{i,s})/\{1+\exp(\delta_{j,k,0}+\sum_{s=1}^{p}\delta_{j,k,s}X_{i,s})\}^2$. Let $\widehat{\boldsymbol{\theta}}$ be the estimator of $\boldsymbol{\theta}$ and $\boldsymbol{S}$ denotes the estimated variance-covariance matrix of $\widehat{\boldsymbol{\theta}}$. Then the estimator of AME_r is $\widehat{AME}_r = (1/n)\sum_{i=1}^{n}\varphi_{r(j,k)}(\boldsymbol{X}_i,\widehat{\boldsymbol{\theta}})$, and the standard error can be calculated by the Delta method. Specifically, the standard error of AME_r can be calculated as,

$$\sqrt{[(1/n)\nabla_{\boldsymbol{\theta}}\sum_{i=1}^{n}\varphi_{r(j,k)}(\boldsymbol{X}_i,\boldsymbol{\theta})]^\top_{\boldsymbol{\theta}=\widehat{\boldsymbol{\theta}}}\,\boldsymbol{S}\,[(1/n)\nabla_{\boldsymbol{\theta}}\sum_{i=1}^{n}\varphi_{r(j,k)}(\boldsymbol{X}_i,\boldsymbol{\theta})]_{\boldsymbol{\theta}=\widehat{\boldsymbol{\theta}}}},$$

where $\nabla_\theta(\bullet) \equiv \partial(\bullet)/\partial\boldsymbol{\theta}$.

For the motivating data example on photosynthesis, we have used the above technique to calculate the marginal effect of the predictors (genetic markers and the environmental factor) on the correlation. Table S6 contains the estimate and 95% CI of the average marginal effects (AMEs) of candidate loci on correlations between phenotypes. For example, the AME of Marker 1 on the correlation between ϕ_{II} and $ECSt$ is estimated to be -0.32 (95% CI: $-0.50, -0.13$) when the marker allele changes from AA to BB. Likewise, the AME of E on the correlation between $NPQt$ and $ECSt$ is estimated to be -0.51 (95% CI: $-0.69, -0.32$).

A.7 Implementation in `R`

To implement our proposed method, we have developed an `R` function named `CMPLE.R`, which is available on GitHub at `https://github.com/ChattoAbhijnan/CMPLE`. This code calculates estimates and standard errors of correlation and standard deviation parameters using the pairwise composite likelihood method. It also provides the p-value and lower and upper limits of the 95% confidence interval. While the original data supporting our study's findings are accessible from the MSU-DOE Plant Research Laboratory, access is limited due to licensing restrictions. Thus, we offer a demonstration example with simulated data (emulating scenario 2) for software implementation.

Input arguments for the function `CMPLE.R`:

`p`: Number of covariates.

`q`: Number of responses.

`mydata`: Data frame containing the covariates followed by the responses in this particular order.

`epsilon`: Threshold for the MM optimization scheme (sum of the absolute relative difference of the parameter estimates between subsequent iterations). We suggest using 0.001.

Output of function `CMPLE.R`:

`out1`= Parameter estimates (first $q*(p+1)$ entries are α parameters, followed by the δ parameters). The first $(p+1)$ parameters of α represent the regression parameters of the standard deviation for the first response, and so on. α can be identified from the labeling of the regression parameters of the standard deviation of the response variables. Likewise, the first $(p+1)$ parameters of δ represent the regression parameters of the pairwise correlation of the response variables and δ can be identified from the labeling of the regression parameters of the pairwise correlation of the response variables.

`out2`= Standard error of parameter estimates (In the same order as out1).

`out3`= A Data frame containing parameter names, estimates, standard error, p-value, and lower and upper limits of the 95% confidence interval.

We refer the readers to the following example code to analyze scenario 2. Specifically, `Data_generation1.R` simulates a data set with p=2 and q=4 for a sample size of n=600. Although, our code works efficiently with reasonable choice of (p, q).

```
> p=2
> q=4
> source("Data_generation1.R")
> head(mydata)
  x1 x2          Y1         Y2        Y3         Y4
1  0  0 -0.22105935 -14.287588 0.1867165 -0.6210162
2  0  1 -0.03701442  -2.837098 5.0161852  0.4388920
3  1  0  0.40403794   6.175764 5.2597804 -0.2438239
4  0  0  0.42709613  14.766235 5.6979028 -0.1072630
5  0  0  0.29515631   5.801195 1.4461312  0.1854944
6  0  1  0.27591000  -7.302657 1.6672484  0.1338266
> source("CMPLE.R")
> results<-CMPLE(mydata,p=2,q=4,epsilon = 0.001)
> results$out3
    Parameter Estimates Std_error P.value   Lower_ci   Upper_ci
1   alpha_1,0     -0.96      0.05    0.00      -1.06      -0.86
2   alpha_1,1      0.95      0.06    0.00       0.83       1.07
3   alpha_1,2      0.29      0.06    0.00       0.17       0.41
4   alpha_2,0      2.03      0.05    0.00       1.93       2.13
5   alpha_2,1      0.14      0.06    0.01       0.02       0.26
6   alpha_2,2     -0.52      0.06    0.00      -0.64      -0.40
7   alpha_3,0      1.02      0.05    0.00       0.92       1.12
8   alpha_3,1      0.32      0.06    0.00       0.20       0.44
```

9	alpha_3,2	0.13	0.06	0.02	0.01	0.25
10	alpha_4,0	-1.05	0.05	0.00	-1.15	-0.95
11	alpha_4,1	-0.40	0.06	0.00	-0.52	-0.28
12	alpha_4,2	1.00	0.06	0.00	0.88	1.12
13	delta_1,2,0	0.31	0.13	0.02	0.06	0.56
14	delta_1,2,1	0.62	0.15	0.00	0.33	0.91
15	delta_1,2,2	0.86	0.15	0.00	0.57	1.15
16	delta_1,3,0	0.56	0.13	0.00	0.31	0.81
17	delta_1,3,1	0.11	0.16	0.50	-0.20	0.42
18	delta_1,3,2	0.24	0.16	0.12	-0.07	0.55
19	delta_1,4,0	0.20	0.15	0.17	-0.09	0.49
20	delta_1,4,1	0.17	0.16	0.28	-0.14	0.48
21	delta_1,4,2	-0.34	0.16	0.03	-0.65	-0.03
22	delta_2,3,0	0.13	0.15	0.38	-0.16	0.42
23	delta_2,3,1	0.95	0.17	0.00	0.62	1.28
24	delta_2,3,2	-0.48	0.17	0.00	-0.81	-0.15
25	delta_2,4,0	0.30	0.14	0.03	0.03	0.57
26	delta_2,4,1	0.46	0.15	0.00	0.17	0.75
27	delta_2,4,2	-1.03	0.16	0.00	-1.34	-0.72
28	delta_3,4,0	-0.10	0.13	0.44	-0.35	0.15
29	delta_3,4,1	0.34	0.16	0.04	0.03	0.65
30	delta_3,4,2	-0.13	0.16	0.43	-0.44	0.18

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Table S1: Results of the simulation study for scenario 1 with $n = 261$, $p = 2$, $q = 4$. All entries of the table except for the true parameter values are multiplied by 100. Par: Parameter, SD: standard deviation, SE: standard error, CP: 95% coverage probability, RMSE: root mean squared error

Par	True	Bias	SD	SE	CP	RMSE	Par	True	Bias	SD	SE	CP	RMSE
$\alpha_{1,0}$	-1.9	-0.9	8.0	7.4	93.8	8.0	$\alpha_{3,0}$	-1.3	-0.1	7.8	7.5	93.2	7.8
$\alpha_{1,1}$	-0.4	0.1	8.9	8.5	93.6	8.9	$\alpha_{3,1}$	-0.2	0.1	8.6	8.6	96.2	8.6
$\alpha_{1,2}$	0.3	-0.1	9.1	8.5	93.0	9.1	$\alpha_{3,2}$	0	-0.9	9.1	8.6	94.0	9.1
$\alpha_{2,0}$	-1.7	0.3	7.8	7.4	92.4	7.8	$\alpha_{4,0}$	-1.4	-0.2	7.9	7.4	92.2	7.9
$\alpha_{2,1}$	-0.4	-1.0	8.8	8.5	93.8	8.9	$\alpha_{4,1}$	0	0	9.2	8.5	92.4	9.2
$\alpha_{2,2}$	0	-0.6	8.9	8.5	93.6	8.9	$\alpha_{4,2}$	0	-0.4	8.9	8.6	93.4	8.9
$\delta_{1,2,0}$	-0.7	-0.4	21.2	20.9	94.2	21.2	$\delta_{2,3,0}$	0	-0.1	22.3	21.2	93.6	22.3
$\delta_{1,2,1}$	-0.8	0.2	24.6	24.5	95.8	24.6	$\delta_{2,3,1}$	0	0.5	26.9	24.5	92.0	26.8
$\delta_{1,2,2}$	0	0.1	25.0	24.1	94.8	25.0	$\delta_{2,3,2}$	0	0.3	25.2	24.6	93.8	25.2
$\delta_{1,3,0}$	1.2	1.3	21.3	21.4	94.6	21.3	$\delta_{2,4,0}$	1.1	1.5	20.9	20.9	93.8	20.9
$\delta_{1,3,1}$	0	-0.9	24.9	24.6	94.6	24.9	$\delta_{2,4,1}$	0	-1.5	24.8	24.0	95.0	24.8
$\delta_{1,3,2}$	0	-0.1	25.5	24.6	94.4	25.5	$\delta_{2,4,2}$	-0.9	-0.2	24.9	24.5	95.6	24.9
$\delta_{1,4,0}$	0	-0.1	22.2	21.1	93.6	22.1	$\delta_{3,4,0}$	0	0.8	22.4	21.2	94.4	22.4
$\delta_{1,4,1}$	0	0.7	25.5	24.3	91.8	25.4	$\delta_{3,4,1}$	0	-1.3	26.1	24.6	93.0	26.1
$\delta_{1,4,2}$	0.6	0.1	24.9	24.6	95.0	24.9	$\delta_{3,4,2}$	0	-0.2	25.4	24.6	95.0	25.4

Table S2: Results of the simulation study for scenario 2 with $n = 600$, $p = 2$, $q = 4$. All entries except for the true parameter values of the table are multiplied by 100. Par: Parameter, SD: standard deviation, SE: standard error, CP: 95% coverage probability, RMSE: root mean squared error

Par	True	Bias	SD	SE	CP	RMSE	Par	True	Bias	SD	SE	CP	RMSE
$\alpha_{1,0}$	-1.0	-0.1	5.1	4.9	94.8	5.1	$\alpha_{3,0}$	1.0	-0.6	5.1	4.9	94.8	5.1
$\alpha_{1,1}$	1.0	0.1	5.7	5.6	94.2	5.7	$\alpha_{3,1}$	0.3	0.4	5.4	5.7	97.0	5.4
$\alpha_{1,2}$	0.2	0	5.7	5.7	94.6	5.7	$\alpha_{3,2}$	0.1	0.3	5.7	5.7	95.0	5.7
$\alpha_{2,0}$	2.0	-0.7	5.0	4.9	93.6	5.1	$\alpha_{4,0}$	-1.0	-0.4	5.3	5.0	92.4	5.3
$\alpha_{2,1}$	0.2	0.2	5.7	5.6	94.4	5.7	$\alpha_{4,1}$	-0.5	0.2	5.4	5.7	96.4	5.4
$\alpha_{2,2}$	-0.5	0.5	5.8	5.7	94.2	5.9	$\alpha_{4,2}$	1.0	0	5.8	5.7	95.4	5.8
$\delta_{1,2,0}$	0.2	0.1	14.0	13.9	93.4	14.0	$\delta_{2,3,0}$	-0.1	0.4	13.7	14.0	94.4	13.7
$\delta_{1,2,1}$	0.5	-0.7	15.6	15.9	95.0	15.6	$\delta_{2,3,1}$	1.0	1.0	15.9	16.2	94.8	16.0
$\delta_{1,2,2}$	1.0	1.2	16.8	16.2	95.6	16.8	$\delta_{2,3,2}$	-0.2	-1.0	15.9	15.8	94.4	15.9
$\delta_{1,3,0}$	0.2	0.7	13.7	14.1	95.6	13.7	$\delta_{2,4,0}$	0.2	0.4	15.1	14.1	94.2	15.1
$\delta_{1,3,1}$	0.2	-1.1	16.3	16.2	94.2	16.3	$\delta_{2,4,1}$	0.5	-0.5	16.6	15.9	95.0	16.6
$\delta_{1,3,2}$	0.5	-0.7	16.4	16.2	94.8	16.4	$\delta_{2,4,2}$	-1.0	0	16.6	16.2	94.2	16.6
$\delta_{1,4,0}$	0.2	0.1	14.0	14.2	95.4	14.0	$\delta_{3,4,0}$	-0.1	0.1	14.2	14.1	94.2	14.2
$\delta_{1,4,1}$	0.2	-0.4	16.2	16.2	94.4	16.2	$\delta_{3,4,1}$	0.2	-0.1	16.5	16.2	95.6	16.5
$\delta_{1,4,2}$	-0.5	1.2	15.9	16.3	96.6	16.0	$\delta_{3,4,2}$	-0.2	0.7	16.4	16.2	94.8	16.4

Table S3: Simulation results for scenario 4 with $n = 1000$, $p = 10$, $q = 4$. All entries except for the true parameter values of the table are multiplied by 100. Par: Parameter, SD: standard deviation, DOP: direct optimization, MM: minorize-maximize

		DOP		MM				DOP		MM	
Par	True	Bias	SD	Bias	SD	Par	True	Bias	SD	Bias	SD
$\alpha_{1,0}$	−1.0	−0.2	9.2	−0.3	9.2	$\alpha_{3,0}$	0.0	−0.3	9.8	−0.3	9.8
$\alpha_{1,1}$	1.0	0.6	6.0	0.6	6.0	$\alpha_{3,1}$	0.3	0.8	6.2	0.8	6.2
$\alpha_{1,2}$	0.2	0.6	6.5	0.7	6.5	$\alpha_{3,2}$	0.1	−0.2	7.3	−0.2	7.3
$\alpha_{1,3}$	−0.4	0.3	6.5	0.3	6.5	$\alpha_{3,3}$	0.0	0.4	6.3	0.4	6.3
$\alpha_{1,4}$	0.3	−0.5	7.2	−0.5	7.2	$\alpha_{3,4}$	−0.2	−0.2	6.4	−0.1	6.4
$\alpha_{1,5}$	0.0	0.0	6.6	0.0	6.6	$\alpha_{3,5}$	0.1	0.2	5.8	0.2	5.8
$\alpha_{1,6}$	−0.5	0.5	5.4	0.6	5.4	$\alpha_{3,6}$	−0.2	−0.6	6.6	−0.6	6.6
$\alpha_{1,7}$	−0.3	0.5	7.0	0.5	6.9	$\alpha_{3,7}$	1.0	0.3	6.7	0.3	6.7
$\alpha_{1,8}$	0.1	−0.3	6.3	−0.2	6.3	$\alpha_{3,8}$	−1.0	0.4	5.5	0.4	5.5
$\alpha_{1,9}$	−0.4	0.6	6.5	0.6	6.5	$\alpha_{3,9}$	−0.1	1.0	6.1	1.0	6.1
$\alpha_{1,10}$	1.0	0.3	6.7	0.3	6.7	$\alpha_{3,10}$	0.2	0.1	6.9	0.2	6.9
$\alpha_{2,0}$	2.0	1.6	9.1	1.6	9.1	$\alpha_{4,0}$	−1.0	0.0	9.1	0.0	9.1
$\alpha_{2,1}$	0.2	−0.7	5.4	−0.7	5.4	$\alpha_{4,1}$	−0.5	1.3	5.7	1.2	5.7
$\alpha_{2,2}$	−0.5	0.0	7.4	0.1	7.4	$\alpha_{4,2}$	0.0	0.3	6.0	0.3	5.9
$\alpha_{2,3}$	−0.4	−0.3	6.3	−0.3	6.3	$\alpha_{4,3}$	0.3	1.2	6.0	1.2	6.0
$\alpha_{2,4}$	0.0	−0.9	5.9	−0.9	5.9	$\alpha_{4,4}$	−0.2	0.1	7.4	0.1	7.4
$\alpha_{2,5}$	0.3	−0.4	5.9	−0.4	5.9	$\alpha_{4,5}$	−0.2	0.2	6.4	0.2	6.4
$\alpha_{2,6}$	0.0	0.0	6.1	0.0	6.1	$\alpha_{4,6}$	0.2	0.0	5.7	0.0	5.7
$\alpha_{2,7}$	0.3	0.4	5.8	0.4	5.8	$\alpha_{4,7}$	0.0	−0.2	6.8	−0.1	6.8
$\alpha_{2,8}$	0.2	0.6	6.1	0.6	6.1	$\alpha_{4,8}$	0.0	0.8	5.9	0.8	5.8
$\alpha_{2,9}$	−0.4	−0.2	6.3	−0.2	6.3	$\alpha_{4,9}$	0.6	−0.7	6.2	−0.7	6.3
$\alpha_{2,10}$	0.0	0.2	5.5	0.2	5.6	$\alpha_{4,10}$	−0.5	−0.5	6.6	−0.5	6.6

Table S3: Simulation results for scenario 4 with $n = 1000$, $p = 10$, $q = 4$. All entries except for the true parameter values of the table are multiplied by 100. Par: Parameter, SD: standard deviation, DOP: direct optimization, MM: minorize-maximize

		DOP		MM				DOP		MM	
Par	True	Bias	SD	Bias	SD	Par	True	Bias	SD	Bias	SD
$\delta_{1,2,0}$	0.2	0.1	30.3	−0.2	29.9	$\delta_{2,3,0}$	0.0	0.8	30.6	0.6	30.5
$\delta_{1,2,1}$	0.5	0.4	19.0	0.5	19.0	$\delta_{2,3,1}$	0.0	−4.6	19.3	−4.5	19.4
$\delta_{1,2,2}$	0.0	2.2	18.8	2.3	18.7	$\delta_{2,3,2}$	−0.2	−0.1	19.3	−0.1	19.3
$\delta_{1,2,3}$	−0.7	−2.3	18.2	−2.2	18.2	$\delta_{2,3,3}$	0.0	−0.2	19.4	−0.2	19.5
$\delta_{1,2,4}$	0.3	1.1	17.5	1.2	17.5	$\delta_{2,3,4}$	0.0	−0.1	18.8	−0.1	18.9
$\delta_{1,2,5}$	0.0	−3.4	17.3	−3.4	17.5	$\delta_{2,3,5}$	0.0	−3.6	17.7	−3.6	17.7
$\delta_{1,2,6}$	−0.8	0.3	20.8	0.3	20.9	$\delta_{2,3,6}$	0.0	5.3	19.9	5.4	19.9
$\delta_{1,2,7}$	0.1	5.2	19.7	5.2	19.7	$\delta_{2,3,7}$	−0.3	2.8	19.3	2.6	19.5
$\delta_{1,2,8}$	0.0	−0.4	15.5	−0.4	15.5	$\delta_{2,3,8}$	0.2	−3.8	16.3	−3.6	16.4
$\delta_{1,2,9}$	0.1	−1.5	19.9	−1.5	20.0	$\delta_{2,3,9}$	0.0	0.1	20.3	0.2	20.3
$\delta_{1,2,10}$	0.2	−1.1	20.7	−0.9	20.7	$\delta_{2,3,10}$	0.0	−1.0	20.1	−0.9	20.1
$\delta_{1,3,0}$	0.5	1.8	30.3	1.4	29.9	$\delta_{2,4,0}$	0.3	0.5	30.6	0.4	30.8
$\delta_{1,3,1}$	0.2	−0.5	20.9	−0.4	21.0	$\delta_{2,4,1}$	0.0	−1.8	19.5	−1.9	19.6
$\delta_{1,3,2}$	0.5	5.1	17.7	5.2	17.7	$\delta_{2,4,2}$	1.0	−2.9	19.9	−3.0	19.7
$\delta_{1,3,3}$	0.0	−4.5	19.3	−4.3	19.2	$\delta_{2,4,3}$	0.4	0.2	18.0	0.3	17.8
$\delta_{1,3,4}$	0.2	1.9	21.0	2.1	21.0	$\delta_{2,4,4}$	−0.3	−1.5	15.6	−1.6	15.7
$\delta_{1,3,5}$	−0.6	−5.9	19.1	−5.8	19.2	$\delta_{2,4,5}$	0.5	2.9	17.6	3.0	17.5
$\delta_{1,3,6}$	0.0	−3.4	17.8	−3.3	17.7	$\delta_{2,4,6}$	0.3	0.5	19.9	0.6	20.1
$\delta_{1,3,7}$	−0.3	0.0	19.2	0.1	19.2	$\delta_{2,4,7}$	0.1	1.9	18.4	1.9	18.4
$\delta_{1,3,8}$	0.2	−3.0	18.8	−2.9	18.8	$\delta_{2,4,8}$	−0.6	−2.1	17.6	−1.9	17.5
$\delta_{1,3,9}$	0.4	2.1	18.4	2.3	18.2	$\delta_{2,4,9}$	0.6	−1.6	18.4	−1.5	18.3
$\delta_{1,3,10}$	−0.2	2.0	18.2	2.0	18.2	$\delta_{2,4,10}$	−0.1	1.0	17.3	0.8	17.1
$\delta_{1,4,0}$	1.0	1.2	30.3	1.1	29.9	$\delta_{3,4,0}$	−1.0	2.7	30.4	3.2	30.0
$\delta_{1,4,1}$	0.2	0.0	18.9	−0.1	18.9	$\delta_{3,4,1}$	0.2	−4.9	19.4	−5.1	19.1
$\delta_{1,4,2}$	−0.5	4.5	21.1	4.3	21.0	$\delta_{3,4,2}$	−0.2	0.1	19.4	−0.2	19.5
$\delta_{1,4,3}$	−0.2	−0.4	20.2	−0.3	20.0	$\delta_{3,4,3}$	−0.1	0.0	18.2	−0.1	18.2
$\delta_{1,4,4}$	0.5	3.1	16.5	3.3	16.7	$\delta_{3,4,4}$	0.2	−3.1	18.0	−3.2	18.0
$\delta_{1,4,5}$	0.1	−0.5	19.0	−0.5	19.2	$\delta_{3,4,5}$	0.6	1.1	19.4	1.0	19.4
$\delta_{1,4,6}$	−0.1	−0.4	20.8	−0.4	21.1	$\delta_{3,4,6}$	−0.1	0.1	21.6	0.1	21.5
$\delta_{1,4,7}$	−0.1	−1.2	20.5	−1.1	20.5	$\delta_{3,4,7}$	0.0	1.3	19.9	0.9	19.4
$\delta_{1,4,8}$	0.0	1.5	17.9	1.5	17.9	$\delta_{3,4,8}$	0.2	−1.0	20.3	−0.8	20.0
$\delta_{1,4,9}$	−0.1	−3.5	18.6	−3.5	18.6	$\delta_{3,4,9}$	0.3	−0.9	20.3	−0.9	20.1
$\delta_{1,4,10}$	−0.2	0.3	19.1	0.4	19.1	$\delta_{3,4,10}$	−0.2	1.6	19.0	1.4	18.8

Table S4: Estimates of the standard deviation parameters based on the two co-localized markers selected through QTL mapping including main effect + two-way interaction effect. Here, M1: Marker 1, M2: Marker 2, E: Environment, I: Intercept

	ϕ_{II}		NPQ_t		qL		ECS_t	
I	-2.61	$(-2.77, -2.45)$	-0.48	$(-0.56, -0.40)$	-2.20	$(-2.36, -2.04)$	-3.11	$(-3.44, -2.78)$
M1	0.20	$(0.02, 0.38)$	-0.01	$(-0.13, 0.11)$	-0.03	$(-0.23, 0.17)$	0.07	$(-0.32, 0.46)$
M2	-0.03	$(-0.23, 0.17)$	0.20	$(0.02, 0.38)$	0.34	$(0.14, 0.54)$	-0.13	$(-0.44, 0.18)$
E	0.10	$(-0.12, 0.32)$	0.33	$(0.09, 0.57)$	-0.19	$(-0.46, 0.08)$	-0.09	$(-0.42, 0.24)$
M1 × M2	-0.22	$(-0.44, 0.01)$	-0.24	$(-0.49, 0.01)$	-0.37	$(-0.64, -0.10)$	-0.24	$(-0.57, 0.09)$
M1 × E	-0.44	$(-0.68, -0.20)$	-0.63	$(-0.90, -0.36)$	0.38	$(0.09, 0.67)$	0.27	$(-0.06, 0.60)$
M2 × E	0.52	$(0.30, 0.74)$	0.85	$(0.58, 1.12)$	-0.50	$(-0.79, -0.21)$	0.05	$(-0.28, 0.38)$

Table S5: Estimates of the pairwise correlation parameters on the two co-localized markers selected through QTL mapping incorporating main effect + two-way interaction effect. Here, M1: Marker 1, M2: Marker 2, E: Environment, I: Intercept

	ϕ_{II}&NPQ_t		ϕ_{II}&qL		ϕ_{II}&ECS_t		NPQ_t&qL		NPQ_t&ECS_t		ECS_t&qL	
I	-1.19	$(-1.54, -0.84)$	1.82	$(1.41, 2.23)$	0.17	$(-0.34, 0.68)$	0.43	$(0.02, 0.86)$	1.01	$(0.65, 1.35)$	1.12	$(0.59, 1.61)$
M1	-1.57	$(-2.04, -1.11)$	0.83	$(0.30, 1.36)$	-0.20	$(-0.81, 0.41)$	-1.71	$(-2.24, -1.18)$	-0.83	$(-1.34, -0.32)$	-0.93	$(-1.56, -0.33)$
M2	1.92	$(1.31, 2.53)$	0.15	$(-0.42, 0.72)$	0.58	$(-0.09, 1.25)$	1.65	$(0.94, 2.36)$	0.74	$(0.11, 1.37)$	0.58	$(-0.07, 1.23)$
E	-1.19	$(-1.80, -0.58)$	-0.25	$(-0.81, 0.35)$	-0.10	$(-0.75, 0.55)$	-0.87	$(-1.50, -0.24)$	-1.10	$(-1.71, -0.49)$	-0.90	$(-1.63, -0.17)$
M1 × M2	-0.73	$(-1.36, -0.10)$	-0.99	$(-1.68, -0.30)$	-0.82	$(-1.55, -0.09)$	-0.26	$(-0.99, 0.47)$	0.17	$(-0.54, 0.88)$	-0.11	$(-0.85, 0.63)$
M1 × E	2.74	$(2.11, 3.37)$	-0.08	$(-0.79, 0.63)$	-0.31	$(-1.04, 0.42)$	2.26	$(1.55, 2.97)$	1.93	$(1.24, 2.62)$	0.91	$(0.13, 1.69)$
M2 × E	-2.47	$(-3.12, -1.82)$	-0.25	$(-0.98, 0.48)$	0.63	$(-0.10, 1.36)$	-1.70	$(-2.41, -0.99)$	-2.09	$(-2.78, -1.40)$	-0.69	$(-1.49, 0.11)$

Table S6: Average marginal effect estimates and 95% confidence interval in parentheses of the pairwise correlations between phenotypes based on predictors. Here, M1: Marker 1, M2: Marker 2, E: Environment

	M1		M2		E	
ϕ_{II}&NPQ_t	-0.11	$(-0.27, 0.04)$	0.03	$(-0.06, 0.12)$	-0.16	$(-0.25, -0.07)$
ϕ_{II}&qL	0.08	$(-0.07, 0.23)$	-0.08	$(-0.17, -0.01)$	-0.08	$(-0.17, 0.01)$
ϕ_{II}&ECS_t	-0.32	$(-0.50, -0.13)$	0.18	$(0.02, 0.37)$	0.08	$(-0.11, 0.27)$
NPQ_t&qL	-0.26	$(-0.48, -0.05)$	0.11	$(-0.09, 0.31)$	-0.20	$(-0.41, -0.01)$
NPQ_t&ECS_t	0.06	$(-0.11, 0.23)$	-0.06	$(-0.23, 0.11)$	-0.50	$(-0.69, -0.32)$
qL&ECS_t	-0.24	$(-0.40, -0.08)$	0.01	$(-0.20, 0.19)$	-0.22	$(-0.41, -0.03)$

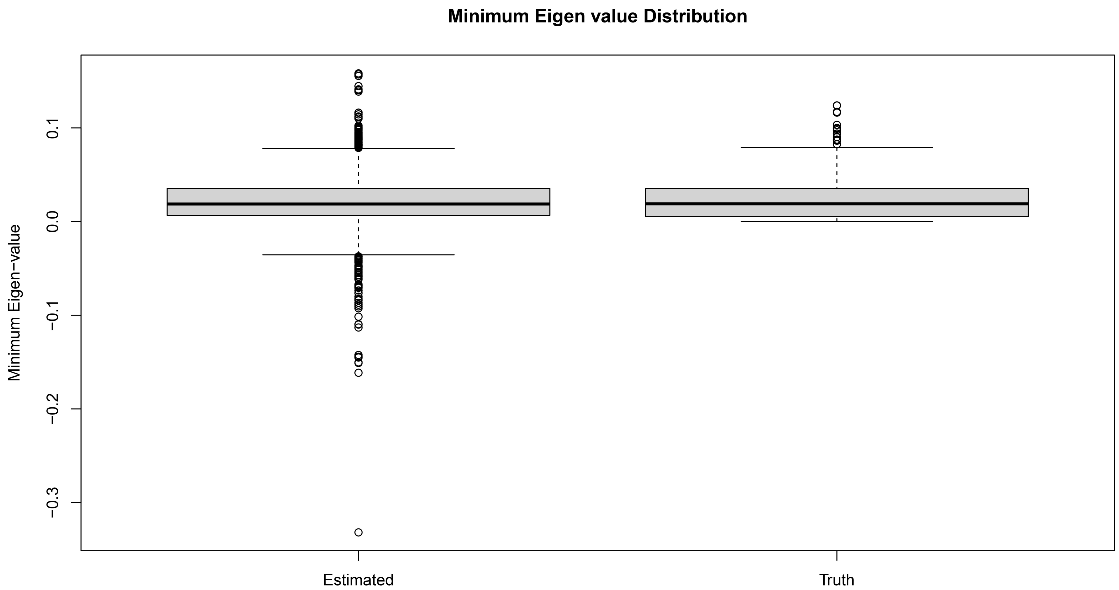

Figure 3: Boxplot of minimum eigen values based on 100 simulated datasets with p =10, q=4 (Emulating scenario 4)

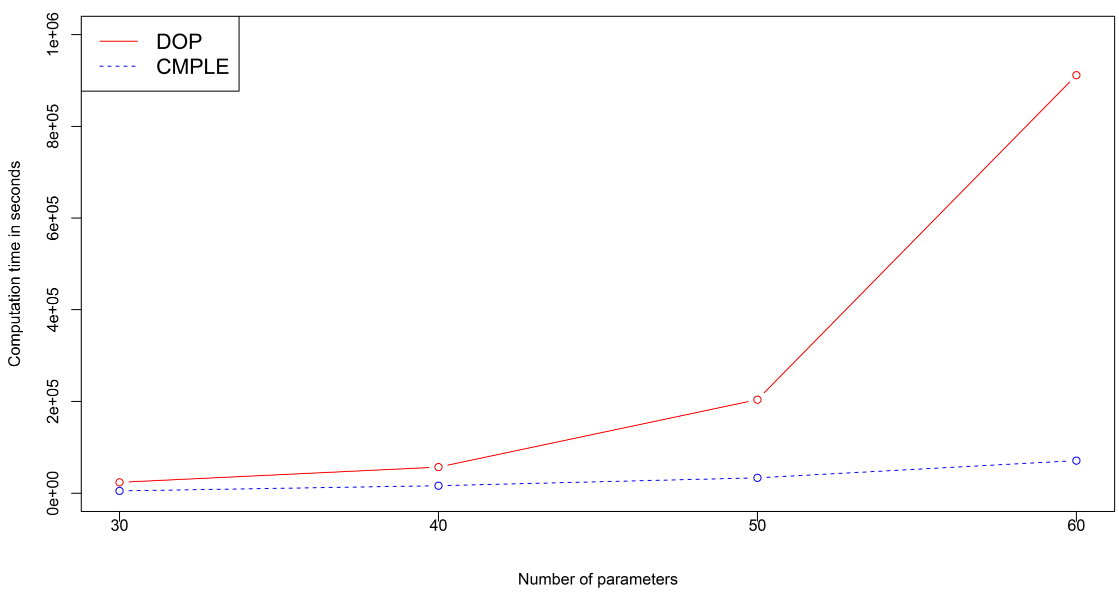

Figure 4: Average computational time comparison between CMPLE and direct optimization method (DOP) for 100 simulations

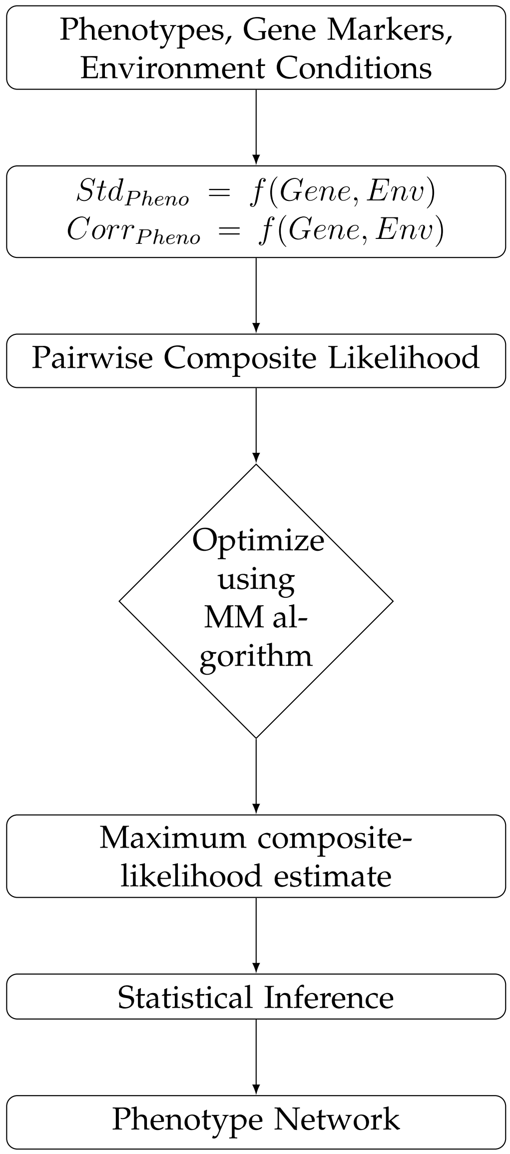

Figure 5: Correlation Modeling Under Pairwise Likelihood Estimation (CMPLE) workflow