

Additional file 1

Details of the algebraic derivations of the formulas in the main text

Algebraic derivation of expression (1)

Let $K = 2^t$ be the number of possible haplotypes, at locus i , for a sliding window of t markers.

Let $\mathbb{1}_{\{u_{QTL,c_1,c_2}=1\}}$ and $\mathbb{1}_{\{u_{QTL,c_1,c_2}=0\}}$ be the following indicator functions:

$$\mathbb{1}_{\{u_{QTL,c_1,c_2}=1\}} = \begin{cases} 1 & \text{if } (c_1, c_2) \text{ have identical alleles at the QTL} \\ 0 & \text{else} \end{cases}$$

$$\mathbb{1}_{\{u_{QTL,c_1,c_2}=0\}} = \begin{cases} 1 & \text{if } (c_1, c_2) \text{ have non-identical alleles at the QTL} \\ 0 & \text{else} \end{cases}$$

We have:

$$\begin{aligned} d_1(\mathbf{M}^{\mathcal{P},i}, \mathbf{M}^{QTL}) &= \frac{1}{4n^2} \sum_{c_1=1}^{2n} \sum_{c_2=1}^{2n} |s_{i,c_1,c_2}^{\mathcal{P}} - u_{QTL,c_1,c_2}| \\ &= \frac{1}{4n^2} \sum_{c_1=1}^{2n} \sum_{c_2=1}^{2n} \mathbb{1}_{\{u_{QTL,c_1,c_2}=1\}} |s_{i,c_1,c_2}^{\mathcal{P}} - 1| + \frac{1}{4n^2} \sum_{c_1=1}^{2n} \sum_{c_2=1}^{2n} \mathbb{1}_{\{u_{QTL,c_1,c_2}=0\}} |s_{i,c_1,c_2}^{\mathcal{P}} - 0| \end{aligned}$$

Let E_{h_p} be the set of chromosome segments carrying haplotype h_p ($p \in \{1, \dots, K\}$) at locus i . We

have:

$$\begin{aligned} d_1(\mathbf{M}^{\mathcal{P},i}, \mathbf{M}^{QTL}) &= \frac{1}{4n^2} \sum_{c_1=1}^{2n} \sum_{c_2=1}^{2n} \sum_{p=1}^K \mathbb{1}_{\{c_1 \in E_{h_p}\}} \sum_{q=1}^K \mathbb{1}_{\{c_2 \in E_{h_q}\}} \mathbb{1}_{\{u_{QTL,c_1,c_2}=1\}} |s_{i,c_1,c_2}^{\mathcal{P}} - 1| \\ &\quad + \frac{1}{4n^2} \sum_{c_1=1}^{2n} \sum_{c_2=1}^{2n} \sum_{p=1}^K \mathbb{1}_{\{c_1 \in E_{h_p}\}} \sum_{q=1}^K \mathbb{1}_{\{c_2 \in E_{h_q}\}} \mathbb{1}_{\{u_{QTL,c_1,c_2}=0\}} |s_{i,c_1,c_2}^{\mathcal{P}} - 0| \end{aligned}$$

where $\mathbb{1}_{\{c_1 \in E_{h_p}\}}$ and $\mathbb{1}_{\{c_2 \in E_{h_q}\}}$ are the indicator functions of the events $\{c_1 \in E_{h_p}\}$ and $\{c_2 \in E_{h_q}\}$ respectively. Indeed $\sum_{p=1}^K \mathbb{1}_{\{c_1 \in E_{h_p}\}}$ and $\sum_{q=1}^K \mathbb{1}_{\{c_2 \in E_{h_q}\}}$ are always equal to one. $d_1(\mathbf{M}^{\mathcal{P},i}, \mathbf{M}^{QTL})$ can thus be expressed as:

$$\begin{aligned} d_1(\mathbf{M}^{\mathcal{P},i}, \mathbf{M}^{QTL}) &= \sum_{p=1}^K \sum_{q=1}^K \frac{1}{4n^2} \sum_{c_1=1}^{2n} \sum_{c_2=1}^{2n} \mathbb{1}_{\{u_{QTL,c_1 \in E_{h_p}, c_2 \in E_{h_q}} = 1\}} |s_{i,h_p,h_q}^{\mathcal{P}} - 1| \\ &+ \sum_{p=1}^K \sum_{q=1}^K \frac{1}{4n^2} \sum_{c_1=1}^{2n} \sum_{c_2=1}^{2n} \mathbb{1}_{\{u_{QTL,c_1 \in E_{h_p}, c_2 \in E_{h_q}} = 0\}} |s_{i,h_p,h_q}^{\mathcal{P}} - 0| \end{aligned}$$

where $\frac{1}{4n^2} \sum_{c_1=1}^{2n} \sum_{c_2=1}^{2n} \mathbb{1}_{\{u_{QTL,c_1 \in E_{h_p}, c_2 \in E_{h_q}} = 1\}} = f(c_1 \in E_{h_p}, c_2 \in E_{h_q}, \text{identical alleles at the QTL})$ is the frequency of chromosome segments, at locus i , carrying h_p and h_q and having identical alleles at the QTL. Since $\{c_1 \in E_{h_p}\}$ and $\{c_2 \in E_{h_q}\}$ are independent events we have:

$$f(c_1 \in E_{h_p}, c_2 \in E_{h_q}, \text{identical alleles at the QTL}) = p_{i,h_p,h_q}^{QTL} f_{i,h_p} f_{i,h_q}$$

where p_{i,h_p,h_q}^{QTL} is the proportion of identical alleles at the QTL by the couples of chromosomes carrying h_p and h_q at position i . f_{i,h_p} and f_{i,h_q} are the frequencies of haplotypes h_p and h_q at position i respectively.

Similarly we have:

$$\begin{aligned} \frac{1}{4n^2} \sum_{c_1=1}^{2n} \sum_{c_2=1}^{2n} \mathbb{1}_{\{u_{QTL,c_1 \in E_{h_p}, c_2 \in E_{h_q}} = 0\}} &= f(c_1 \in E_{h_p}, c_2 \in E_{h_q}, \text{non-identical alleles at the QTL}) \\ &= (1 - p_{i,h_p,h_q}^{QTL}) f_{i,h_p} f_{i,h_q} \end{aligned}$$

Consequently $d_1(\mathbf{M}^{\mathcal{P},i}, \mathbf{M}^{QTL})$ can be written as (1), i.e.

$$d_1(\mathbf{M}^{\mathcal{P},i}, \mathbf{M}^{QTL}) = \sum_{p=1}^K \sum_{q=1}^K f_{i,h_p} f_{i,h_q} \left[p_{i,h_p,h_q}^{QTL} (1 - s_{i,h_p,h_q}^{\mathcal{P}}) + (1 - p_{i,h_p,h_q}^{QTL}) s_{i,h_p,h_q}^{\mathcal{P}} \right] \quad (1)$$

Algebraic derivation of expression (2)

Let $(n_{h_p})_{1 \leq p \leq K}$ be the counts of the possible haplotypes at a tested position i . And let $(n_{h_p a_l})_{\substack{1 \leq p \leq K \\ 1 \leq l \leq 2}}$ be the counts of the $2K$ possible haplotypes defined between i and a QTL. Expression (1) can be rewritten as:

$$\begin{aligned} d_1(\mathbf{M}^{\mathcal{P},i}, \mathbf{M}^{QTL}) &= \sum_{p=1}^K \sum_{q=1}^K \frac{n_{h_p}}{2n} \frac{n_{h_q}}{2n} \left[\frac{[n_{h_p a_1} n_{h_q a_1} + n_{h_p a_2} n_{h_q a_2}]}{n_{h_p} n_{h_q}} (1 - s_{i,h_p,h_q}^{\mathcal{P}}) \right. \\ &\quad \left. + \left(\frac{n_{h_p} n_{h_q} - [n_{h_p a_1} n_{h_q a_1} + n_{h_p a_2} n_{h_q a_2}]}{n_{h_p} n_{h_q}} \right) s_{i,h_p,h_q}^{\mathcal{P}} \right] \\ &= \sum_{p=1}^K \sum_{q=1}^K \left[\left[f_{i,h_p a_1}^{QTL} f_{i,h_q a_1}^{QTL} + f_{i,h_p a_2}^{QTL} f_{i,h_q a_2}^{QTL} \right] (1 - s_{i,h_p,h_q}^{\mathcal{P}}) \right. \\ &\quad \left. + \left(\frac{(n_{h_p a_1} + n_{h_p a_2})(n_{h_q a_1} + n_{h_q a_2})}{4n^2} - f_{i,h_p a_1}^{QTL} f_{i,h_q a_1}^{QTL} - f_{i,h_p a_2}^{QTL} f_{i,h_q a_2}^{QTL} \right) s_{i,h_p,h_q}^{\mathcal{P}} \right] \end{aligned}$$

which simplifies to (2):

$$\begin{aligned} d_1(\mathbf{M}^{\mathcal{P},i}, \mathbf{M}^{QTL}) &= \sum_{p=1}^K \sum_{q=1}^K \left[\left[f_{i,h_p a_1}^{QTL} f_{i,h_q a_1}^{QTL} + f_{i,h_p a_2}^{QTL} f_{i,h_q a_2}^{QTL} \right] (1 - s_{i,h_p,h_q}^{\mathcal{P}}) \right. \\ &\quad \left. + \left[f_{i,h_p a_2}^{QTL} f_{i,h_q a_1}^{QTL} + f_{i,h_p a_1}^{QTL} f_{i,h_q a_2}^{QTL} \right] s_{i,h_p,h_q}^{\mathcal{P}} \right] \quad (2) \end{aligned}$$

Algebraic derivation of expression (3)

Let $f_{i,h_p a_1}^{QTL} = f_{i,h_p} f_{a_1} + \Delta_{\mathbf{p}} = \alpha_p + \Delta_{\mathbf{p}}$ and $f_{i,h_p a_2}^{QTL} = f_{i,h_p} f_{a_2} - \Delta_{\mathbf{p}} = \tilde{\alpha}_p - \Delta_{\mathbf{p}}$. Note that we have $\sum_{p=1}^K \Delta_{\mathbf{p}} = \sum_{p=1}^K (f_{i,h_p a_1}^{QTL} - f_{i,h_p} f_{a_1}) = f_{a_1} - f_{a_1} \sum_{p=1}^K f_{i,h_p} = 0$. Replacing the haplotype frequencies in

expression (2) with the expressions including the α_p , $\tilde{\alpha}_p$ and $\Delta_{\mathbf{p}}$ terms (same for the frequencies depending on the α_q , $\tilde{\alpha}_q$ and $\Delta_{\mathbf{q}}$ terms) gives:

$$\begin{aligned}
d(\mathbf{M}^{\mathcal{P},i}, \mathbf{M}^{QTL}) = & \sum_{p=1}^k \left[-4s_{i,h_p,h_p}^{\mathcal{P}} \Delta_{\mathbf{p}}^2 + \left[\alpha_p - \tilde{\alpha}_p + 4s_{i,h_p,h_p}^{\mathcal{P}} (\tilde{\alpha}_p - \alpha_p) + \sum_{q \neq p}^k (\alpha_q - \tilde{\alpha}_q) \right] \Delta_{\mathbf{p}} \right. \\
& + \alpha_p^2 + \tilde{\alpha}_p^2 + s_{i,h_p,h_p}^{\mathcal{P}} (-\alpha_p^2 - \tilde{\alpha}_p^2 + 2\alpha_p \tilde{\alpha}_p) + \sum_{q \neq p}^k \alpha_p \alpha_q + \tilde{\alpha}_p \tilde{\alpha}_q \\
& + \sum_{q \neq p}^k s_{i,h_p,h_q}^{\mathcal{P}} \left(-4\Delta_{\mathbf{p}} \Delta_{\mathbf{q}} + 2(\tilde{\alpha}_p - \alpha_p) \Delta_{\mathbf{q}} + 2(\tilde{\alpha}_q - \alpha_q) \Delta_{\mathbf{p}} \right. \\
& \left. \left. - \alpha_p \alpha_q - \tilde{\alpha}_p \tilde{\alpha}_q + \tilde{\alpha}_p \alpha_q + \alpha_p \tilde{\alpha}_q \right) \right] \quad (*)
\end{aligned}$$

Replacing $\Delta_{\mathbf{q}}$ with $-\Delta_{\mathbf{p}} - \sum_{l \neq p,q}^K \Delta_{\mathbf{l}}$ (since $\sum_{p=1}^k \Delta_{\mathbf{p}} = 0$) in (*) finally gives:

$$\begin{aligned}
d_1(\mathbf{M}^{\mathcal{P},i}, \mathbf{M}^{QTL}) = & \sum_{p=1}^K \left[4 \left(\sum_{q \neq p}^K s_{i,h_p,h_q}^{\mathcal{P}} - s_{i,h_p,h_p}^{\mathcal{P}} \right) \Delta_{\mathbf{p}}^2 + \left[\alpha_p - \tilde{\alpha}_p + 4s_{i,h_p,h_p}^{\mathcal{P}} (\tilde{\alpha}_p - \alpha_p) \right. \right. \\
& \left. \left. + \sum_{q \neq p}^K \left(\alpha_q - \tilde{\alpha}_q + s_{i,h_p,h_q}^{\mathcal{P}} \left(4 \sum_{l \neq p,q}^K \Delta_{\mathbf{l}} + 2(\alpha_p - \tilde{\alpha}_p) + 2(\tilde{\alpha}_q - \alpha_q) \right) \right) \right] \Delta_{\mathbf{p}} \right. \\
& + \alpha_p^2 + \tilde{\alpha}_p^2 + s_{i,h_p,h_p}^{\mathcal{P}} (-\alpha_p^2 - \tilde{\alpha}_p^2 + 2\alpha_p \tilde{\alpha}_p) + \sum_{q \neq p}^K \alpha_p \alpha_q + \tilde{\alpha}_p \tilde{\alpha}_q \\
& \left. + \sum_{q \neq p}^K s_{i,h_p,h_q}^{\mathcal{P}} \left(2(\alpha_p - \tilde{\alpha}_p) \sum_{l \neq p,q}^K \Delta_{\mathbf{l}} - \alpha_p \alpha_q - \tilde{\alpha}_p \tilde{\alpha}_q + \tilde{\alpha}_p \alpha_q + \alpha_p \tilde{\alpha}_q \right) \right]
\end{aligned}$$

Hence $d_1(\mathbf{M}^{\mathcal{P},i}, \mathbf{M}^{QTL})$ can be expressed as (3):

$$\begin{aligned}
d_1(\mathbf{M}^{\mathcal{P},i}, \mathbf{M}^{QTL}) = & \sum_{p=1}^K \left[4 \left(\sum_{q \neq p}^K s_{i,h_p,h_q}^{\mathcal{P}} - s_{i,h_p,h_p}^{\mathcal{P}} \right) \Delta_{\mathbf{p}}^2 + \Psi_{p\mathbf{q}}^{\mathcal{P}}(\Delta_{l \neq p,q}) \Delta_{\mathbf{p}} + \Phi_{pq}^{\mathcal{P}}(\Delta_{l \neq p,q}) \right] \\
= & \xi^{\mathcal{P}}(\Delta_{\mathbf{1}}, \dots, \Delta_{\mathbf{K}}) \quad (3)
\end{aligned}$$

Algebraic derivation of expression (4)

Expression (4) is obtained directly from expression (3) for $s_{i,h_p,h_p}^{\mathcal{P}} = 1$ and $s_{i,h_p,h_q}^{\mathcal{P}} = 0$ when $\mathcal{P} = \text{IBS}_{\text{hap}}$.

Algebraic derivation of expressions (5) and (6)

Considering that only two haplotypes exist among the K possible ones is the same as setting $K = 2$. Expression (5) can be obtained directly by reducing expression (4) for the case where $K = 2$. However another derivation is given here so as to exhibit other properties, such as a lower bound, for the matrix distance. For $K = 2$ expression (2) becomes:

$$\begin{aligned} d_1(\mathbf{M}^{\mathcal{P},i}, \mathbf{M}^{QTL}) &= (f_{i,h_1a_1}^{QTL})^2 + (f_{i,h_1a_2}^{QTL})^2 - s_{i,h_1,h_1}^{\mathcal{P}} (f_{i,h_1a_1}^{QTL} - f_{i,h_1a_2}^{QTL})^2 \\ &\quad + 2(f_{i,h_1a_1}^{QTL} f_{i,h_2a_1}^{QTL} + f_{i,h_1a_2}^{QTL} f_{i,h_2a_2}^{QTL})(1 - s_{i,h_1,h_2}^{\mathcal{P}}) \\ &\quad + 2(f_{i,h_1a_2}^{QTL} f_{i,h_2a_1}^{QTL} + f_{i,h_1a_1}^{QTL} f_{i,h_2a_2}^{QTL}) s_{i,h_1,h_2}^{\mathcal{P}} \\ &\quad - s_{i,h_2,h_2}^{\mathcal{P}} (f_{i,h_2a_1}^{QTL} - f_{i,h_2a_2}^{QTL})^2 + (f_{i,h_2a_1}^{QTL})^2 + (f_{i,h_2a_2}^{QTL})^2 \end{aligned}$$

and the frequencies in expression (2) can be written as:

$$f_{i,h_1a_1}^{QTL} = f_{i,h_1} f_{a_1} + \Delta_1 = \alpha_1 + \Delta_1$$

$$f_{i,h_1a_2}^{QTL} = f_{i,h_1} f_{a_2} - \Delta_1 = \tilde{\alpha}_1 - \Delta_1$$

$$f_{i,h_2a_1}^{QTL} = f_{i,h_2} f_{a_1} - \Delta_1 = \alpha_2 - \Delta_1$$

$$f_{i,h_2a_2}^{QTL} = f_{i,h_2} f_{a_2} + \Delta_1 = \tilde{\alpha}_2 + \Delta_1$$

Note that Δ_1 , in this case, can be expressed as $\Delta_1 = f_{i,h_1a_1}^{QTL} f_{i,h_2a_2}^{QTL} - f_{i,h_1a_2}^{QTL} f_{i,h_2a_1}^{QTL}$ with its maximum and minimum value given by $\frac{1}{4}$ and $-\frac{1}{4}$ respectively. The maximum value of Δ_1 is given by $f_{i,h_1a_1}^{QTL} =$

$f_{i,h_2a_2}^{QTL} = \frac{1}{2}$ and $f_{i,h_1a_2}^{QTL} = f_{i,h_2a_1}^{QTL} = 0$, and its minimum value is given by $f_{i,h_1a_1}^{QTL} = f_{i,h_2a_2}^{QTL} = 0$ and $f_{i,h_1a_2}^{QTL} = f_{i,h_2a_1}^{QTL} = \frac{1}{2}$. Replacing the haplotype frequencies in $d_1(\mathbf{M}^{\mathcal{P},i}, \mathbf{M}^{QTL})$ with the expressions including the $\alpha_1, \tilde{\alpha}_1, \tilde{\alpha}_2, \alpha_2$ and Δ_1 terms gives:

$$\begin{aligned}
d_1(\mathbf{M}^{\mathcal{P},i}, \mathbf{M}^{QTL}) &= [-4s_{i,h_1,h_1}^{\mathcal{P}} - 4s_{i,h_2,h_2}^{\mathcal{P}} + 8s_{i,h_1,h_2}^{\mathcal{P}}] \Delta_1^2 \\
&\quad + [4s_{i,h_1,h_1}^{\mathcal{P}}(\tilde{\alpha}_1 - \alpha_1) + 4s_{i,h_2,h_2}^{\mathcal{P}}(\alpha_2 - \tilde{\alpha}_2) - 4s_{i,h_1,h_2}^{\mathcal{P}}(\tilde{\alpha}_1 + \alpha_2 - (\alpha_1 + \tilde{\alpha}_2))] \Delta_1 \\
&\quad - s_{i,h_1,h_1}^{\mathcal{P}}(\tilde{\alpha}_1 - \alpha_1)^2 - s_{i,h_2,h_2}^{\mathcal{P}}(\alpha_2 - \tilde{\alpha}_2)^2 + 2s_{i,h_1,h_2}^{\mathcal{P}}(\tilde{\alpha}_1 - \alpha_1)(\alpha_2 - \tilde{\alpha}_2) \\
&\quad + (\alpha_1 + \alpha_2)^2 + (\tilde{\alpha}_2 + \tilde{\alpha}_1)^2 \\
&= \xi^{\mathcal{P}}(\Delta_1)
\end{aligned}$$

Hence $d_1(\mathbf{M}^{\mathcal{P},i}, \mathbf{M}^{QTL})$ can be expressed as:

$$\xi^{\mathcal{P}}(\Delta_1) = [-4s_{i,h_1,h_1}^{\mathcal{P}} - 4s_{i,h_2,h_2}^{\mathcal{P}} + 8s_{i,h_1,h_2}^{\mathcal{P}}] \Delta_1^2 + \Psi^{\mathcal{P}} \Delta_1 + \Phi^{\mathcal{P}} \quad (5)$$

For the extreme values of Δ_1 we have:

$$\xi^{\mathcal{P}}\left(\frac{1}{4}\right) = \xi^{\mathcal{P}}\left(-\frac{1}{4}\right) = \frac{1}{2} + \frac{1}{2}s_{i,h_1,h_2}^{\mathcal{P}} - \frac{1}{4}(s_{i,h_1,h_1}^{\mathcal{P}} + s_{i,h_2,h_2}^{\mathcal{P}})$$

This quantity can also be obtained simply from expression (2), when $K = 2$, by replacing $f_{i,h_1a_1}^{QTL}$, $f_{i,h_2a_2}^{QTL}$, $f_{i,h_1a_2}^{QTL}$ and $f_{i,h_2a_1}^{QTL}$ by their corresponding values for the maximum and minimum value of Δ_1 .

For $\Delta_1 = \frac{1}{4}$ we have:

$$\begin{aligned}
d_1(\mathbf{M}^{\mathcal{P},i}, \mathbf{M}^{QTL}) &= \left(\left(\frac{1}{2}\right)^2 + 0^2\right) - s_{i,h_1,h_1}^{\mathcal{P}}\left(\frac{1}{2} - 0\right)^2 + 2\left(\frac{1}{2} \cdot 0 + 0 \cdot \frac{1}{2}\right)(1 - s_{i,h_1,h_2}^{\mathcal{P}}) \\
&\quad + 2\left(0 \cdot 0 + \frac{1}{2} \cdot \frac{1}{2}\right)s_{i,h_1,h_2}^{\mathcal{P}} - s_{i,h_2,h_2}^{\mathcal{P}}\left(0 - \frac{1}{2}\right)^2 + \left(0^2 + \left(\frac{1}{2}\right)^2\right) \\
&= \frac{1}{2} + \frac{1}{2}s_{i,h_1,h_2}^{\mathcal{P}} - \frac{1}{4}(s_{i,h_1,h_1}^{\mathcal{P}} + s_{i,h_2,h_2}^{\mathcal{P}}) \\
&= \xi^{\mathcal{P}}\left(\frac{1}{4}\right)
\end{aligned}$$

In the same manner we can show that $\xi^{\mathcal{P}}\left(-\frac{1}{4}\right) = \xi^{\mathcal{P}}\left(\frac{1}{4}\right)$ since the squares and the products of the frequencies in expression (2) when $K = 2$ are symmetric. $\frac{1}{2} + \frac{1}{2}s_{i,h_1,h_2}^{\mathcal{P}} - \frac{1}{4}(s_{i,h_1,h_1}^{\mathcal{P}} + s_{i,h_2,h_2}^{\mathcal{P}})$ is greater or equal to $\frac{1}{2}s_{i,h_1,h_2}^{\mathcal{P}}$ since the maximum possible value of $s_{i,h_1,h_1}^{\mathcal{P}}$ and $s_{i,h_2,h_2}^{\mathcal{P}}$ is equal to one. Hence if haplotypes h_1 and h_2 share allele similarity $s_{i,h_1,h_2}^{\mathcal{P}}$ will be positive and $\xi^{\mathcal{P}}\left(-\frac{1}{4}\right) = \xi^{\mathcal{P}}\left(\frac{1}{4}\right) \in [\frac{1}{2}s_{i,h_1,h_2}^{\mathcal{P}}, 1]$. For $\mathcal{P} = \text{IBS}_{\text{hap}}$, i.e. $s_{i,h_1,h_1}^{\mathcal{P}} = s_{i,h_2,h_2}^{\mathcal{P}} = 1$ and $s_{i,h_1,h_2}^{\mathcal{P}} = 0$, we have $\xi^{\mathcal{P}}\left(-\frac{1}{4}\right) = \xi^{\mathcal{P}}\left(\frac{1}{4}\right) = 0$. Note that for $\mathcal{P} = \text{IBS}_{\text{hap}}$ $\xi^{\mathcal{P}}(\mathbf{\Delta}_1)$ becomes:

$$\begin{aligned} \xi^{\text{IBS}_{\text{hap}}}(\mathbf{\Delta}_1) &= -8\mathbf{\Delta}_1^2 + 4[(\tilde{\alpha}_1 - \alpha_1) + (\alpha_2 - \tilde{\alpha}_2)]\mathbf{\Delta}_1 - (\tilde{\alpha}_1 - \alpha_1)^2 - (\alpha_2 - \tilde{\alpha}_2)^2 \\ &\quad + (\alpha_1 + \alpha_2)^2 + (\tilde{\alpha}_2 + \tilde{\alpha}_1)^2 \end{aligned} \quad (6)$$

Thus differentiating $\xi^{\text{IBS}_{\text{hap}}}$ with respect to $\mathbf{\Delta}_1$ gives:

$$\mathbf{\Delta}_1^* = \frac{\tilde{\alpha}_1 - \alpha_1 + \alpha_2 - \tilde{\alpha}_2}{4} = \frac{(2f_{a_1} - 1)(1 - 2f_{i,h_1})}{4}$$

The minimum of $\mathbf{\Delta}_1^*$, which is equal to $-\frac{1}{4}$, is given by either $f_{a_1} = f_{i,h_1} = 1$ or $f_{a_1} = f_{i,h_1} = 0$. Its maximum value, which is equal to $\frac{1}{4}$, is given by either $f_{a_1} = 0$ and $f_{i,h_1} = 1$ or $f_{a_1} = 1$ and $f_{i,h_1} = 0$. Hence $\mathbf{\Delta}_1^*$ takes its minimum and maximum values when both the tested locus and the QTL are monomorphic.

Algebraic derivation of the matrix distance for a multiallelic QTL

For S distinct alleles at the QTL expression (2) generalizes to:

$$d_1(\mathbf{M}^{\mathcal{P},i}, \mathbf{M}^{\text{QTL}}) = \sum_{p=1}^K \sum_{q=1}^K \left[(1 - s_{i,h_p,h_q}^{\mathcal{P}}) \sum_{l=1}^S f_{i,h_p a_l}^{\text{QTL}} f_{i,h_q a_l}^{\text{QTL}} + s_{i,h_p,h_q}^{\mathcal{P}} \sum_{l=1}^S \sum_{m \neq l}^S f_{i,h_p a_l}^{\text{QTL}} f_{i,h_q a_m}^{\text{QTL}} \right] \quad (7)$$

For $\mathcal{P} = \text{IBS}_{\text{hap}}$ expression (7) becomes:

$$d_1(\mathbf{M}^{\text{IBShap},i}, \mathbf{M}^{\text{QTL}}) = \sum_{p=1}^K \sum_{l=1}^S \sum_{m \neq l}^S f_{i,h_p a_l}^{\text{QTL}} f_{i,h_p a_m}^{\text{QTL}} + \sum_{p=1}^K \sum_{l=1}^S \sum_{q \neq p}^K f_{i,h_p a_l}^{\text{QTL}} f_{i,h_q a_l}^{\text{QTL}} \quad (7)$$

Let $\Delta_{\mathbf{pl}} = f_{i,h_p a_l}^{\text{QTL}} - f_{i,h_p} f_{a_l} = f_{i,h_p a_l}^{\text{QTL}} - \alpha_{pl}$, which is equivalent to $f_{i,h_p a_l}^{\text{QTL}} = \alpha_{pl} + \Delta_{\mathbf{pl}}$. Note that:

$$D_{i,\text{QTL}}^2 = \sum_{p=1}^K \sum_{l=1}^S (f_{i,h_p a_l}^{\text{QTL}} - f_{i,h_p} \cdot f_{a_l})^2 = \sum_{p=1}^K \sum_{l=1}^S \Delta_{\mathbf{pl}}^2$$

Since $\sum_{p=1}^K \Delta_{\mathbf{pl}} = 0$ we have $\sum_{q \neq p}^K \Delta_{\mathbf{ql}} = -\Delta_{\mathbf{pl}}$ and $\sum_{m \neq l}^S \Delta_{\mathbf{pm}} = -\Delta_{\mathbf{pl}}$. Replacing the haplotype frequencies in expression (7) with the LD coefficients and the product of frequencies terms, and subsequently replacing $\sum_{q \neq p}^K \Delta_{\mathbf{ql}}$ and $\sum_{m \neq l}^S \Delta_{\mathbf{pm}}$ with $-\Delta_{\mathbf{pl}}$, gives:

$$\begin{aligned} d_1(\mathbf{M}^{\text{IBShap},i}, \mathbf{M}^{\text{QTL}}) &= \sum_{p=1}^K \sum_{l=1}^S \left[-2\Delta_{\mathbf{pl}}^2 + \left(\Psi_{pl}^{\text{IBShap},(1)} + \Psi_{pl}^{\text{IBShap},(2)} \right) \Delta_{\mathbf{pl}} \right. \\ &\quad \left. + \left(\Phi_{pl}^{\text{IBShap},(1)} + \Phi_{pl}^{\text{IBShap},(2)} \right) \right] \\ &= \xi^{\text{IBShap}}(\Delta_{\mathbf{11}}, \Delta_{\mathbf{12}}, \dots, \Delta_{\mathbf{KS}}) \end{aligned}$$

As for expression (3) the general behavior of the matrix distance for continuous predictors in $[0, 1]$, as function of LD coefficients, is unspecifiable for the multiallelic QTL case. Hence we did not express the matrix distance, here in the multiallelic QTL case, for continuous predictors in $[0, 1]$.