

Newton-Raphson algorithm in estimating r in Scenario 4 in clonal F_1 progenies

For linkage phase I, using the theoretical frequencies of genotypes in Table 5, the likelihood function was given in Eq. (S1).

$$L = \frac{n!}{n_1! \cdots n_{12}!} \left[\frac{1}{4} (1-r)^2 \right]^{n_1+n_{12}} \left[\frac{1}{4} r(1-r) \right]^{n_4+n_{6;7}+n_9} \left[\frac{1}{2} r(1-r) \right]^{n_2+n_{11}} \times \left[\frac{1}{4} r^2 \right]^{n_3+n_{10}} \left[\frac{1}{4} (1-2r+2r^2) \right]^{n_5+n_8}, \quad (S1)$$

where n_1 - n_{12} were observed sample sizes of the 12 genotypes, n_{ij} is sum of n_i to n_j , and n was the total sample size (i.e. $n=n_{1:12}$). The logarithm of the likelihood was given in Eq. (S2).

$$\log L = C + (2n_1 + n_2 + n_4 + n_{6;7} + n_9 + n_{11} + 2n_{12}) \log(1-r) + (n_2 + 2n_3 + n_4 + n_{6;7} + n_9 + 2n_{10} + n_{11}) \log r + (n_5 + n_8) \log(1-2r+2r^2) \quad (S2)$$

It is impossible to acquire an analytic MLE of r by solving the likelihood equation. Steps of Newton-Raphson algorithm to acquire a numerical solution of r were shown below.

Step 1: Assuming the initial value of r as 0.00001, and ϵ is the bearable error;

Step 2: Calculating the first derivative $f'(r)$ and the second derivative $f''(r)$ as given in Eq. S3 and S4, respectively.

$$f'(r) = \frac{d \ln L}{dr} = \frac{n_2 + 2n_3 + n_4 + n_{6;7} + n_9 + 2n_{10} + n_{11}}{r} - \frac{2n_1 + n_2 + n_4 + n_{6;7} + n_9 + n_{11} + 2n_{12}}{1-r} + \frac{4r-2}{1-2r+2r^2} (n_5 + n_8) \quad (S3)$$

$$f''(r) = \frac{d^2 \ln L}{d^2 r} = -\frac{n_2 + 2n_3 + n_4 + n_{6:7} + n_9 + 2n_{10} + n_{11}}{r^2} - \frac{2n_1 + n_2 + n_4 + n_{6:7} + n_9 + n_{11} + 2n_{12}}{(1-r)^2} + \frac{8r(1-r)}{(1-2r+2r^2)^2} (n_5 + n_8) \quad (S4)$$

Step 3: Updating r as follows: $r_{i+1} = r_i - f'(r_i)/f''(r_i)$. If $|r_{i+1} - r_i| \leq \varepsilon$ then let $\hat{r} = r_{i+1}$;

Otherwise, let $r_{i+1} = r_i$, and repeat step 2 until $|r_{i+1} - r_i| \leq \varepsilon$.

For linkage phase II, the likelihood function and logarithm likelihood were given in Eq. S5 and S6,

respectively.

$$L = \frac{n!}{n_1! \cdots n_{12}!} \left[\frac{1}{4} (1-r)^2 \right]^{n_4 + n_9} \left[\frac{1}{4} r(1-r) \right]^{n_1 + n_3 + n_{10} + n_{12}} \left[\frac{1}{2} r(1-r) \right]^{n_5 + n_8} \times \left[\frac{1}{4} r^2 \right]^{n_{6:7}} \left[\frac{1}{4} (1-2r+2r^2) \right]^{n_2 + n_{11}} \quad (S5)$$

$$\log L = C + (n_1 + n_3 + 2n_4 + n_5 + n_8 + 2n_9 + n_{10} + n_{12}) \log(1-r) +$$

$$(n_1 + n_3 + n_5 + 2n_{6:7} + n_8 + 2n_{10} + n_{12}) \log r + (n_2 + n_{11}) \log(1-2r+2r^2) \quad (S6)$$

The first derivative $f'(r)$ and the second derivative $f''(r)$ were given in Eq. S7 and S8, respectively.

$$f'(r) = \frac{d \ln L}{dr} = \frac{n_1 + n_3 + n_5 + 2n_{6:7} + n_8 + n_{10} + n_{12}}{r} - + \frac{n_1 + n_3 + 2n_4 + n_5 + n_8 + 2n_9 + n_{10} + n_{12}}{1-r} + \frac{4r-2}{1-2r+2r^2} (n_2 + n_{11}) \quad (S7)$$

$$f''(r) = \frac{d^2 \ln L}{d^2 r} = -\frac{n_1 + n_3 + n_5 + 2n_{6:7} + n_8 + n_{10} + n_{12}}{r^2} - \frac{n_1 + n_3 + 2n_4 + n_5 + n_8 + 2n_9 + n_{10} + n_{12}}{(1-r)^2} + \frac{8r(1-r)}{(1-2r+2r^2)^2} (n_2 + n_{11}) \quad (S8)$$

For linkage phase III, the likelihood function and logarithm likelihood were given in Eq. S9 and S10,

respectively.

$$L = \frac{n!}{n_1! \cdots n_{12}!} \left[\frac{1}{4} (1-r)^2 \right]^{n_{6,7}} \left[\frac{1}{4} r(1-r) \right]^{n_1 + n_3 + n_{10} + n_{12}} \left[\frac{1}{2} r(1-r) \right]^{n_5 + n_8} \times \left[\frac{1}{4} r^2 \right]^{n_4 + n_9} \left[\frac{1}{4} (1-2r+2r^2) \right]^{n_2 + n_{11}} \quad (S9)$$

The logarithm of the likelihood is therefore,

$$\log L = C + (n_1 + n_3 + n_5 + 2n_{6,7} + n_8 + 2n_{10} + n_{12}) \log(1-r) + (n_1 + n_3 + 2n_4 + n_5 + n_8 + 2n_9 + n_{10} + n_{12}) \log r + (n_2 + n_{11}) \log(1-2r+2r^2) \quad (S10)$$

The first derivative $f'(r)$ and the second derivative $f''(r)$ were given in Eq. S11 and S12,

respectively.

$$f'(r) = \frac{d \ln L}{dr} = \frac{n_1 + n_3 + 2n_4 + n_5 + n_8 + 2n_9 + n_{10} + n_{12}}{r} - \frac{n_1 + n_3 + n_5 + 2n_{6,7} + n_8 + n_{10} + n_{12}}{1-r} + \frac{4r-2}{1-2r+2r^2} (n_2 + n_{11}) \quad (S11)$$

$$f''(r) = \frac{d^2 \ln L}{d^2 r} = -\frac{n_1 + n_3 + 2n_4 + n_5 + n_8 + 2n_9 + n_{10} + n_{12}}{r^2} - \frac{n_1 + n_3 + n_5 + 2n_{6,7} + n_8 + n_{10} + n_{12}}{(1-r)^2} + \frac{8r(1-r)}{(1-2r+2r^2)^2} (n_2 + n_{11}) \quad (S12)$$

For linkage phase IV, the likelihood function and logarithm likelihood were given in Eq. S13 and S14,

respectively.

$$L = \frac{n!}{n_1! \cdots n_{12}!} \left[\frac{1}{4} (1-r)^2 \right]^{n_3 + n_{10}} \left[\frac{1}{4} r(1-r) \right]^{n_4 + n_{6,7} + n_9} \left[\frac{1}{2} r(1-r) \right]^{n_2 + n_{11}} \times \cdot$$

$$\left[\frac{1}{4}r^2\right]^{n_1+n_{12}} \left[\frac{1}{4}(1-2r+2r^2)\right]^{n_5+n_8} \quad (\text{S13})$$

$$\begin{aligned} \log L = & C + (n_2 + 2n_3 + n_4 + n_{6:7} + n_9 + 2n_{10} + n_{11}) \log(1-r) + \\ & (2n_1 + n_2 + n_4 + n_{6:7} + n_9 + n_{11} + 2n_{12}) \log r + (n_5 + n_8) \log(1-2r+2r^2) \end{aligned} \quad (\text{S14})$$

The first derivative $f'(r)$ and the second derivative $f''(r)$ were given in Eq. S15 and S16, respectively.

$$\begin{aligned} f'(r) = \frac{d \ln L}{dr} = & \frac{2n_1 + n_2 + n_4 + n_{6:7} + n_9 + n_{11} + 2n_{12}}{r} - \\ & \frac{n_2 + 2n_3 + n_4 + n_{6:7} + n_9 + 2n_{10} + n_{11}}{1-r} + \frac{4r-2}{1-2r+2r^2} (n_5 + n_8) \end{aligned} \quad (\text{S15})$$

$$\begin{aligned} f''(r) = \frac{d^2 \ln L}{d^2 r} = & -\frac{2n_1 + n_2 + n_4 + n_{6:7} + n_9 + n_{11} + 2n_{12}}{r^2} - \\ & \frac{n_2 + 2n_3 + n_4 + n_{6:7} + n_9 + 2n_{10} + n_{11}}{(1-r)^2} + \frac{8r(1-r)}{(1-2r+2r^2)^2} (n_5 + n_8) \end{aligned} \quad (\text{S16})$$