

Algorithm

The posterior distribution for are $\boldsymbol{\theta} = (\mu, \nu, E, E_0, A, b_x, b_y)$ given the data is

$$\pi(\boldsymbol{\theta}|\mathbf{c}, \mathbf{x}, \mathbf{y}, \mathbf{n}) \propto L(\boldsymbol{\theta}; \mathbf{c}, \mathbf{x}, \mathbf{y}, \mathbf{n})\pi(\boldsymbol{\theta})$$

with the likelihood

$$L(\boldsymbol{\theta}; \mathbf{c}, \mathbf{x}, \mathbf{y}, \mathbf{n}) \propto p(0,0; \mu, \nu)^{n_0} p(0,1; \mu, \nu)^{n_1} \times \\ \left\{ \prod_{j=1}^{n_2} \sum_{i=1}^{m_2 c_0} p(i, c_0; \mu, \nu, E, E_0) \left[\Phi \left(h, iAG_{\tilde{c}_j}, iA^2 G_{\tilde{c}_j} \left(\frac{1-E}{1+E} \right) (G_{\tilde{c}_j} - 1) \right) - \right. \right. \\ \left. \left. \Phi \left(h, iAG_{\tilde{c}_j+\delta}, iA^2 G_{\tilde{c}_j+\delta} \left(\frac{1-E}{1+E} \right) (G_{\tilde{c}_j+\delta} - 1) \right) \right] \right\}$$

where $\Phi(x, \mu, \sigma^2) = \int_{-\infty}^x \phi(s, \mu, \sigma^2) ds$ is the distribution function of the normal distribution. See 'Additional file 1.pdf' for derivation and more details.

The joint prior distribution $\pi(\boldsymbol{\theta})$ is the product of the individual prior distributions given by

$$\begin{aligned} \mu &\sim \Gamma(\alpha_1, \beta_1) \\ \nu &\sim \Gamma(\alpha_2, \beta_2) \\ E &\sim \text{Beta}(\alpha_3, \beta_3) \\ E_1 &\sim \text{Beta}(\alpha_4, \beta_4) \\ \pi(b_x) &\propto 1 \\ \pi(b_y) &\propto 1 \\ \pi(A) &\propto A^{-1} \end{aligned}$$

for values of $\alpha_1, \dots, \alpha_4, \beta_1, \dots, \beta_4$ that reflect prior opinion regarding the associated parameters. See main paper for more details.

The function used to transform $\boldsymbol{\theta}$ to $\boldsymbol{\varphi} = (\mu', \nu', E', E_1', A', b_x, b_y)$ is:

$$\boldsymbol{\varphi} = f(\boldsymbol{\theta}) = \left(\log(\mu), \log(\nu), -\log\left(\frac{1}{E} - 1\right), -\log\left(\frac{1}{E_0} - 1\right), \frac{\log(A)}{\log(1+E)}, b_x, b_y \right), \quad (1)$$

with the inverse given by

$$\boldsymbol{\theta} = f^{-1}(\boldsymbol{\varphi}) = \left(e^{\mu'}, e^{\nu'}, (1 + e^{-E'})^{-1}, (1 + e^{-E_1'})^{-1}, (1 + E')^{A'}, b_x, b_y \right), \quad (2)$$

The posterior in terms of the transformed parameters is given by

$$\pi(\boldsymbol{\varphi}|\mathbf{c}, \mathbf{x}, \mathbf{y}, \mathbf{n}) = \pi(f^{-1}(\boldsymbol{\theta})|\mathbf{c}, \mathbf{x}, \mathbf{y}, \mathbf{n}) \times \mu\nu(1+E)E_1(1-E_1)\log(1+E)A$$

The algorithm for producing the MCMC chain is as follows in which N is the length of the chain:

1. For each combination of $\tilde{E}, \tilde{E}_1$ calculate the initial parameter estimates

$$\tilde{\boldsymbol{\theta}} = \left(\tilde{\mu} = -\log\left(\frac{n_0}{n}\right), \tilde{\nu} = 1, \tilde{E}, \tilde{E}_1, \tilde{A} = h e^{\frac{0.6n_0}{n_0+n}} (1 + \tilde{E}_1)^{-1} (1 + \tilde{E})^{1-\tilde{c}}, \tilde{b}_x, \tilde{b}_y \right)$$

- (a) Transform from $\tilde{\boldsymbol{\theta}}$ to $\tilde{\boldsymbol{\varphi}}$ using Equation (1).

- (b) Estimate the local maximum $\boldsymbol{\varphi}_{\text{mode}}$ using the Nelder-Mead algorithm starting at $\tilde{\boldsymbol{\varphi}}$

2. From the results of step 1 identify the overall mode $\boldsymbol{\varphi}_{\text{mode}}$;

3. Estimate the Hessian matrix $\mathbf{H}$ at $\boldsymbol{\varphi}_{\text{mode}}$, and use the matrix to estimate the covariance matrix $\boldsymbol{\Sigma}_{\text{mode}} = \mathbf{H}^{-1}$. (If $\mathbf{H}$ is not invertible reduce the elements on its diagonal so that it is.)

4. Set $\boldsymbol{\varphi}^{(1)} = \boldsymbol{\varphi}_{\text{mode}}$;

5. For $i = 2 : N$

- (a) Sample u from Uniform(0,1)

- (b) Sample $\boldsymbol{\varphi}^*$ from $N(\boldsymbol{\varphi}^{(i-1)}, \boldsymbol{\Sigma}_{\text{mode}})$

- (c) If

$$u < \min \left\{ 1, \frac{\pi(\boldsymbol{\varphi}^* | \mathbf{c}, \mathbf{x}, \mathbf{y}, \mathbf{n})}{\pi(\boldsymbol{\varphi}^{(i-1)} | \mathbf{c}, \mathbf{x}, \mathbf{y}, \mathbf{n})} \right\}$$

then

$$\boldsymbol{\varphi}^{(i)} = \boldsymbol{\varphi}^*$$

otherwise

$$\boldsymbol{\varphi}^{(i)} = \boldsymbol{\varphi}^{(i-1)}$$

6. Transform values $\boldsymbol{\varphi}^{(1)}, \dots, \boldsymbol{\varphi}^{(N)}$ back to $\boldsymbol{\theta}^{(1)}, \dots, \boldsymbol{\theta}^{(N)}$ using Equations (2).

Steps 3-5 are performed by the R function MCMCmetrop1R from the MCMCpack package.