

Given an observed response sequence  $Y_k^{(t)}$ , and simulated  $\Lambda_{\langle \varepsilon, n_c, \gamma_{CS} \rangle}$  :

$$\mathfrak{L}\left(\Lambda_{\langle \varepsilon, n_c, \gamma_{CS} \rangle} \| Y_k^{(t)}\right) = \prod_{t=1}^{|Y^{(t)}|} f\left(Y_k^{(t)} \| \Lambda_{\langle \varepsilon, n_c, \gamma_{CS} \rangle}\right)$$

$$\text{let } \left\{ \begin{array}{lcl} N & = & 40 \\ \varepsilon & = & -.5, \dots, .5 \\ n_c & = & 10, \dots, 30 \\ \gamma_{CS} & = & 0, \dots, 1 \\ \Lambda_{\langle \varepsilon, n_c, \gamma_{CS} \rangle} & = & \{\Phi, \Theta, \Pi\} \\ \lambda_{\pi}^{(t=1)} & = & P\left(\theta^{(t=1)} = \theta_{\pi}^{(t=1)} | Y_k^{(t=1)}\right) = \pi_i \\ \lambda_i^{(t)} & = & P\left(\theta^{(t)} = \theta_i^{(t)} | Y_k^{(t)}\right) \\ \lambda_j^{(t+1)} & = & P\left(\theta^{(t+1)} = \theta_j^{(t+1)} | Y_k^{(t+1)}\right) \end{array} \right.$$

Assume :

$$\begin{aligned} \forall Y_k^{(t)} \in \{ /bAk/, /dAk/ \} : V(x, y)_{\langle \varepsilon, n_c, \gamma_{CS} \rangle} \vdash \lambda_{\pi ij}^{(t)} \quad \therefore \\ \theta^{(t)} = \arg \max_{\pi ij} \lambda_{\pi ij}^{(t)} \end{aligned}$$

Then the Maximum Likelihood Estimate of the tuple  $\langle \varepsilon, n_c, \gamma_{CS} \rangle$  given  $Y_k^{(t)}$  is defined as :

$$\begin{aligned} \mathfrak{L}\left(\Lambda_{\langle \varepsilon, n_c, \gamma_{CS} \rangle} \| Y_k^{(1)}, Y_k^{(N)}\right) &= \prod_{m=1}^{N-1} \prod_{n=2}^N \left( \phi_{\lambda_j^{(m)} \rightarrow \lambda_j^{(n)}} \theta_{\lambda_j}^{(n)} \pi_i \right) \\ \ln \mathfrak{L}\left(\Lambda_{\langle \varepsilon, n_c, \gamma_{CS} \rangle} \| Y_k^{(1)}, Y_k^{(N)}\right) &= \sum_{m=1}^{N-1} \sum_{n=2}^N \ln \left( \phi_{\lambda_j^{(m)} \rightarrow \lambda_j^{(n)}} \theta_{\lambda_j}^{(n)} \pi_i \right) \quad \therefore \\ \langle \varepsilon, n_c, \gamma_{CS} \rangle_{MLE} &= \arg \max_{\varepsilon, n_c, \gamma_{CS}} \ln \mathfrak{L}\left(\Lambda_{\langle \varepsilon, n_c, \gamma_{CS} \rangle} \| Y_k^{(1)}, Y_k^{(N)}\right) \\ \langle \varepsilon, n_c, \gamma_{CS} \rangle_{MLE} &= \arg \max_{\varepsilon, n_c, \gamma_{CS}} \sum_{n=1}^N \ln P\left(Y_k^{(1)}, Y_k^{(N)} | \Lambda_{\langle \varepsilon, n_c, \gamma_{CS} \rangle}\right) \end{aligned}$$

Box 5.2. Definition of the Maximum Likelihood Estimator used to estimate parameters  $\varepsilon$  and  $\gamma_{CS}$  of the 2D potential model for each observed experimental trial sequence. See text for details.