

Web-based Supplementary Materials for Bayesian variable selection for multistate Markov models with interval-censored data in an ecological momentary assessment of an attempt to quit smoking

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Web Appendix

Web Appendix A: Convergence Stopping Rule

To determine convergence of our proposed method, we set a stopping rule for the absolute value of the difference between the log-likelihood distribution evaluated at the current and next step of the algorithm (Wu, 1983). Formally, the algorithm stops if

$$\left| \ell(\Phi^{(k+1)} | \mathbf{y}) - \ell(\Phi^{(k)} | \mathbf{y}) \right| = \left| \left[Q[\Phi^{(k+1)} | \Phi^{(k)}] - Q[\Phi^{(k)} | \Phi^{(k)}] \right] - \left[R[\Phi^{(k+1)} | \Phi^{(k)}] - R[\Phi^{(k)} | \Phi^{(k)}] \right] \right| \leq \epsilon,$$

where ℓ is the log-likelihood function and ϵ is the stopping rule threshold. The Q-function is described in Eq. 4. To complete the derivation of our stopping rule, we define

$$R[\Phi | \Phi^{(k)}] = \sum_{\gamma} \log(\pi(\gamma | \Phi, \mathbf{y})) \times \pi(\gamma | \Phi^{(k)}, \mathbf{y}) = E_{\gamma | \cdot} \log(\pi(\gamma | \Phi, \mathbf{y})).$$

Due to the hierarchical structure of this model, we assume that

$$\pi(\gamma | \Phi, \mathbf{y}) = \pi(\gamma | \Phi) = \theta^{\sum_{r=1}^p (\gamma_{\lambda,r} + \gamma_{\mu,r})} (1 - \theta)^{2p - \sum_{r=1}^p (\gamma_{\lambda,r} + \gamma_{\mu,r})}. \quad (\text{A.1})$$

Taking the log and conditional expectation of A.1, we show

$$E_{\gamma | \cdot} \log(\pi(\gamma | \Phi)) = \sum_{r=1}^p [E_{\gamma | \cdot}[\gamma_{\lambda,r}] + E_{\gamma | \cdot}[\gamma_{\mu,r}]] \log(\theta) + \left(2p - \sum_{r=1}^p E_{\gamma | \cdot}[\gamma_{\lambda,r}] + E_{\gamma | \cdot}[\gamma_{\mu,r}] \right) \log(1 - \theta).$$

Once the algorithm has converged, the final estimates, $\hat{\Phi}$, maximize Eq. 4.

Web Appendix B: Deterministic Annealing Variant

The deterministic annealing EM algorithm (DAEM) redefines the EM algorithm's objective based on the principle of maximum entropy to reduce the algorithm's dependence on initial values. Instead of maximizing the Q-function, the new objective is to minimize the free energy function at gradually cooler temperatures. For EMVS, this corresponds to maximizing the

negative free energy function

$$-\mathfrak{F}_t(\Phi) = -\mathfrak{U}_t(\Phi) + \frac{1}{t}\mathfrak{S}_t(\Phi) = \frac{1}{t} \log \sum_{\gamma} (\pi(\Phi, \gamma | \mathbf{y}))^t,$$

where $\mathfrak{U}_t(\Phi)$ is the internal energy, $\mathfrak{S}_t(\Phi)$ is the entropy, and $\frac{1}{t}$ is interpreted as the temperature of the annealing process, with $0 < t < 1$. Equivalently, we can maximize $-\mathfrak{F}_t(\Phi)$ by iteratively maximizing the negative internal energy, conditioned on the current estimates of the unknown parameters, $\Phi^{(k)}$ (Ueda and Nakano, 1998). The negative internal energy function is

$$-\mathfrak{U}_t(\Phi | \Phi^{(k)}) = \sum_{\gamma} \log(\pi(\Phi, \gamma | \mathbf{y})) \times \pi(\gamma | \Phi^{(k)})^t \quad (\text{A.2})$$

In application, the annealing process starts with a high temperature (i.e., t close to 0). When the temperature is high, the landscape of $-\mathfrak{F}_t(\Phi)$ is smooth, which prevents the EM algorithm from getting stuck in a local mode early in its iterative process. As the temperature iteratively cools, the effect of the inclusion posterior is strengthened. As a result, local modes begin to appear and the landscape of $-\mathfrak{F}_t(\Phi)$ progressively approaches the true incomplete posterior.

To formulate our ECM algorithm with a deterministic annealing variant, we introduce an annealing loop that regulates the influence of the inclusion posterior and replace Eq. 4 with equation Eq. A.2 in the E-step. The algorithm for this method is

Step 1: Set the initial $\Phi^{(0)}$ and t .

Step 2: Carry out the ECM steps at the current temperature, t , until convergence:

- (a) E-Step: Evaluate $\mathfrak{U}_t \left[\Phi | \Phi^{(k)} \right]$
- (b) CM-steps: Perform steps 1-3 in Section 2.3, replacing Eq. 4 with Eq. A.2.
- (c) Set $k \leftarrow k + 1$

Step 3: Increase t .

Step 4: If $t < 1$, return to step 2 and use the final estimates given the previous t to initiate at the current t . Else, stop.

Here, the conditional expectation is taken with respect to a tempered inclusion posterior distribution. The tempered probabilities of inclusion are calculated as

$$p_{r,t}^* = \frac{\left[\pi(\beta_r^{(k)} | \gamma_r = 1) P(\gamma_r = 1 | \theta^{(k)}) \right]^t}{\left[\pi(\beta_r^{(k)} | \gamma_r = 0) P(\gamma_r = 0 | \theta^{(k)}) \right]^t + \left[\pi(\beta_r^{(k)} | \gamma_r = 1) P(\gamma_r = 1 | \theta^{(k)}) \right]^t}.$$

At each cooling step, t , we find a global mode that is used to initiate the algorithm at the next temperature to find a new global mode. Assuming that the new global mode is close to the previous, the probability of converging at the true global mode is increased. Note that on the final annealing loop iteration ($t = 1$), Eq. 4 matches equation Eq. A.2. Thus, the parameter estimates that maximize the negative free-energy function are equivalent to the posterior mode estimates that maximize the log incomplete posterior. While convergence at the global mode is still not guaranteed, the variant removes the algorithm's dependence on initial parameter values and finds better estimates than the conventional EM algorithm (Ueda and Nakano, 1998).

Web Appendix C: Variance Estimation

We present the closed-form expressions for $\partial^2 Q [\Phi | \hat{\Phi}] / \partial \Phi \partial \Phi'$ and $\text{var}\{\partial \log \pi(\Phi, \gamma | \mathbf{y}) / \partial \Phi | \hat{\Phi}, \mathbf{y}\}$ from Eq. 5 in the main article. For simplicity, we redefine the Q-function as

$$\begin{aligned} Q[\Phi | \Phi^{(k)}] = & C + \sum_{i=1}^m \sum_{j=2}^{n_i} \left[\log P_{y_i(t_{i,j-1}), y_i(t_{i,j})}(\delta_{ij} | \mathbf{x}_{i,j-1}) \right] \\ & + \sum_{r=0}^p -\frac{1}{2} \left\{ \beta_{\lambda,r}^2 E_{\gamma|\cdot} \left[\frac{1}{v_0(1 - \gamma_{\lambda,r}) + v_1 \gamma_{\lambda,r}} \right] + \beta_{\mu,r}^2 E_{\gamma|\cdot} \left[\frac{1}{v_0(1 - \gamma_{\mu,r}) + v_1 \gamma_{\mu,r}} \right] \right\} \\ & + \sum_{r=1}^p E_{\gamma|\cdot} [\gamma_{\lambda,r} + \gamma_{\mu,r}] \log \left(\frac{\theta}{1 - \theta} \right) + (a - 1) \log \theta + (b + 2p - 1) \log(1 - \theta), \end{aligned}$$

where $\mathbf{x}'_{ij} = (1, x_{ij1}, \dots, x_{ijp})$, $\boldsymbol{\gamma}_\lambda = (\gamma_{\lambda,0}, \dots, \gamma_{\lambda,p})$, $\boldsymbol{\gamma}_\mu = (\gamma_{\mu,0}, \dots, \gamma_{\mu,p})$, $\boldsymbol{\beta}'_\lambda = (\lambda_0, \beta_{\lambda,1}, \dots, \beta_{\lambda,p})$, and $\boldsymbol{\beta}'_\mu = (\mu_0, \beta_{\mu,1}, \dots, \beta_{\mu,p})$. By setting $\gamma_{\lambda,0} \equiv 1$ and $\gamma_{\mu,0} \equiv 1$, λ_0 and μ_0 are forced into the

model. The second derivative of the Q-function can be partitioned into

$$\frac{\partial^2 Q[\Phi|\Phi^{(k)}]}{\partial \Phi \partial \Phi'} = \begin{bmatrix} \frac{\partial^2 Q[\Phi|\Phi^{(k)}]}{\partial \beta_\lambda \partial \beta'_\lambda} & \frac{\partial^2 Q[\Phi|\Phi^{(k)}]}{\partial \beta_\lambda \partial \beta'_\mu} & \mathbf{0}_{(p+1) \times 1} \\ \frac{\partial^2 Q[\Phi|\Phi^{(k)}]'}{\partial \beta_\lambda \partial \beta'_\mu} & \frac{\partial^2 Q[\Phi|\Phi^{(k)}]}{\partial \beta_\mu \partial \beta'_\mu} & \mathbf{0}_{(p+1) \times 1} \\ \mathbf{0}_{1 \times (p+1)} & \mathbf{0}_{1 \times (p+1)} & \frac{\partial^2 Q[\Phi|\Phi^{(k)}]}{\partial \theta^2} \end{bmatrix}_{(2p+3) \times (2p+3)}.$$

Due to the complexity of the following derivations, we use multiple substitutions for clarity. Here, major derivations are presented first, and their components are defined after. For instance, second derivatives may be written as functions of first derivatives, which are defined thereafter. We let

$$\begin{aligned} \log P_{y_i(t_{i,j-1}), y_i(t_{i,j})}(\delta_{ij} | \mathbf{x}_{i,j-1}) &= \log(B + AC) I(N, N) + \log(A - AC) I(N, S) \\ &+ \log(A + BC) I(S, S) + \log(B - BC) I(S, N) \\ &- \log(A + B), \end{aligned}$$

where the indicator function $I(y_i(t_{i,j-1}), y_i(t_{i,j}))$ represents the observed transition for subject i from the assessment at time $t_{i,j-1}$ to $t_{i,j}$. Recall that $y_i(t_{i,j})$ is defined as N if the subject is in a non-smoking state and S if the subject is in a smoking state. Here, we set

$$A = \lambda^{i,j-1} = \exp(\mathbf{x}'_{i,j-1} \beta_\lambda),$$

$$B = \mu^{i,j-1} = \exp(\mathbf{x}'_{i,j-1} \beta_\mu),$$

and

$$C = \exp(-(A + B)\delta_{ij}).$$

It is important to note that in the following derivations, A , B , and C depend on i and j , but we suppress their subscripts for ease of reading.

Here, we provide the first derivatives of the Q-function with respect to Φ .

The first derivatives of the Q-function are

$$\begin{aligned} \frac{\partial Q [\Phi | \Phi^{(k)}]}{\partial \beta_\lambda} &= \sum_{i=1}^m \sum_{j=2}^{n_i} \left[\frac{\frac{\partial(B+AC)}{\partial \beta_\lambda}}{(B+AC)} I(N, N) + \frac{\frac{\partial(A-AC)}{\partial \beta_\lambda}}{(A-AC)} I(N, S) \right. \\ &\quad \left. + \frac{\frac{\partial(A+BC)}{\partial \beta_\lambda}}{(A+BC)} I(S, S) + \frac{\frac{\partial(B-BC)}{\partial \beta_\lambda}}{(B-BC)} I(S, N) - \frac{\frac{\partial(A+B)}{\partial \beta_\lambda}}{(A+B)} \right] \\ &\quad - \beta_\lambda \circ \left[E_{\gamma \cdot} \left[\frac{1}{v_0(1-\gamma_\lambda) + v_1\gamma_\lambda} \right] \right], \end{aligned}$$

$$\begin{aligned} \frac{\partial Q [\Phi | \Phi^{(k)}]}{\partial \beta_\mu} &= \sum_{i=1}^m \sum_{j=2}^{n_i} \left[\frac{\frac{\partial(B+AC)}{\partial \beta_\mu}}{(B+AC)} I(N, N) + \frac{\frac{\partial(A-AC)}{\partial \beta_\mu}}{(A-AC)} I(N, S) \right. \\ &\quad \left. + \frac{\frac{\partial(A+BC)}{\partial \beta_\mu}}{(A+BC)} I(S, S) + \frac{\frac{\partial(B-BC)}{\partial \beta_\mu}}{(B-BC)} I(S, N) - \frac{\frac{\partial(A+B)}{\partial \beta_\mu}}{(A+B)} \right] \\ &\quad - \beta_\mu \circ \left[E_{\gamma \cdot} \left[\frac{1}{v_0(1-\gamma_\mu) + v_1\gamma_\mu} \right] \right], \end{aligned}$$

and

$$\frac{\partial Q [\Phi | \Phi^{(k)}]}{\partial \theta} = \sum_{r=1}^p \left[E_{\gamma \cdot} [\gamma_{\lambda,r} + \gamma_{\mu,r}] \left[\frac{1}{\theta} + \frac{1}{1-\theta} \right] \right] + \frac{a-1}{\theta} - \frac{b+2p-1}{1-\theta},$$

where \circ is the component-wise product of two vectors.

Then, the second derivatives of the Q-function are shown to be

$$\begin{aligned} \frac{\partial^2 Q [\Phi | \Phi^{(k)}]}{\partial \beta_\lambda \partial \beta'_\lambda} &= \sum_{i=1}^m \sum_{j=2}^{n_i} \left[\frac{\frac{\partial^2(A+BC)}{\partial \beta_\lambda \partial \beta'_\lambda} (A+BC) - \frac{\partial(A+BC)}{\partial \beta_\lambda} \frac{\partial(A+BC)}{\partial \beta'_\lambda}}{(A+BC)^2} I(S, S) \right. \\ &\quad + \frac{\frac{\partial^2(B+AC)}{\partial \beta_\lambda \partial \beta'_\lambda} (B+AC) - \frac{\partial(B+AC)}{\partial \beta_\lambda} \frac{\partial(B+AC)}{\partial \beta'_\lambda}}{(B+AC)^2} I(N, N) \\ &\quad + \frac{\frac{\partial^2(A-AC)}{\partial \beta_\lambda \partial \beta'_\lambda} (A-AC) - \frac{\partial(A-AC)}{\partial \beta_\lambda} \frac{\partial(A-AC)}{\partial \beta'_\lambda}}{(A-AC)^2} I(N, S) \\ &\quad + \frac{\frac{\partial^2(B-BC)}{\partial \beta_\lambda \partial \beta'_\lambda} (B-BC) - \frac{\partial(B-BC)}{\partial \beta_\lambda} \frac{\partial(B-BC)}{\partial \beta'_\lambda}}{(B-BC)^2} I(S, N) \\ &\quad \left. - \frac{\frac{\partial^2 A}{\partial \beta_\lambda \partial \beta'_\lambda} (A+B) - \frac{\partial A}{\partial \beta_\lambda} \frac{\partial A}{\partial \beta'_\lambda}}{(A+B)^2} \right] - \text{diag} \left(E_{\gamma \cdot} \left[\frac{1}{v_0(1-\gamma_\lambda) + v_1\gamma_\lambda} \right] \right), \end{aligned}$$

$$\begin{aligned} \frac{\partial^2 Q [\Phi | \Phi^{(k)}]}{\partial \beta_\mu \partial \beta'_\mu} &= \sum_{i=1}^m \sum_{j=2}^{n_i} \left[\frac{\frac{\partial^2(A+BC)}{\partial \beta_\mu \partial \beta'_\mu} (A+BC) - \frac{\partial(A+BC)}{\partial \beta_\mu} \frac{\partial(A+BC)}{\partial \beta'_\mu}}{(A+BC)^2} I(S, S) \right. \\ &+ \frac{\frac{\partial^2(B+AC)}{\partial \beta_\mu \partial \beta'_\mu} (B+AC) - \frac{\partial(B+AC)}{\partial \beta_\mu} \frac{\partial(B+AC)}{\partial \beta'_\mu}}{(B+AC)^2} I(N, N) \\ &+ \frac{\frac{\partial^2(A-AC)}{\partial \beta_\mu \partial \beta'_\mu} (A-AC) - \frac{\partial(A-AC)}{\partial \beta_\mu} \frac{\partial(A-AC)}{\partial \beta'_\mu}}{(A-AC)^2} I(N, S) \\ &+ \frac{\frac{\partial^2(B-BC)}{\partial \beta_\mu \partial \beta'_\mu} (B-BC) - \frac{\partial(B-BC)}{\partial \beta_\mu} \frac{\partial(B-BC)}{\partial \beta'_\mu}}{(B-BC)^2} I(S, N) \\ &\left. - \frac{\frac{\partial^2 B}{\partial \beta_\mu \partial \beta'_\mu} (A+B) - \frac{\partial B}{\partial \beta_\mu} \frac{\partial B}{\partial \beta'_\mu}}{(A+B)^2} \right] - \text{diag} \left(E_{\gamma \cdot} \left[\frac{1}{v_0(1-\gamma_\mu) + v_1\gamma_\mu} \right] \right), \end{aligned}$$

$$\begin{aligned} \frac{\partial^2 Q [\Phi | \Phi^{(k)}]}{\partial \beta_\lambda \partial \beta'_\mu} &= \sum_{i=1}^m \sum_{j=2}^{n_i} \left[\frac{\frac{\partial^2(A+BC)}{\partial \beta_\lambda \partial \beta'_\mu} (A+BC) - \frac{\partial(A+BC)}{\partial \beta_\lambda} \frac{\partial(A+BC)}{\partial \beta'_\mu}}{(A+BC)^2} I(S, S) \right. \\ &+ \frac{\frac{\partial^2(B+AC)}{\partial \beta_\lambda \partial \beta'_\mu} (B+AC) - \frac{\partial(B+AC)}{\partial \beta_\lambda} \frac{\partial(B+AC)}{\partial \beta'_\mu}}{(B+AC)^2} I(N, N) \\ &+ \frac{-\frac{\partial^2(B+AC)}{\partial \beta_\lambda \partial \beta'_\mu} (A-AC) - \frac{\partial(A-AC)}{\partial \beta_\lambda} \frac{\partial(A-AC)}{\partial \beta'_\mu}}{(A-AC)^2} I(N, S) \\ &+ \frac{-\frac{\partial^2(A+BC)}{\partial \beta_\lambda \partial \beta'_\mu} (B-BC) - \frac{\partial(B-BC)}{\partial \beta_\lambda} \frac{\partial(B-BC)}{\partial \beta'_\mu}}{(B-BC)^2} I(S, N) \\ &\left. + \frac{\frac{\partial A}{\partial \beta_\lambda} \frac{\partial B}{\partial \beta'_\mu}}{(A+B)^2} \right], \end{aligned}$$

and

$$\frac{\partial^2 Q [\Phi | \Phi^{(k)}]}{\partial \theta^2} = \sum_{r=1}^p \left[E_{\gamma \cdot} [\gamma_{\lambda,r} + \gamma_{\mu,r}] \left[-\frac{1}{\theta^2} + \frac{1}{(1-\theta)^2} \right] \right] - \frac{a-1}{\theta^2} - \frac{b+2p-1}{(1-\theta)^2}.$$

where $\text{diag}(\cdot)$ represents a diagonal matrix. The second derivatives in these equations are shown below.

The second derivatives of $(A+BC)$ are

$$\frac{\partial^2(A+BC)}{\partial \beta_\lambda \partial \beta'_\lambda} = \frac{\partial^2 A}{\partial \beta_\lambda \partial \beta'_\lambda} (1 - BC\delta_{ij}) + BC\delta_{ij}^2 \frac{\partial A}{\partial \beta_\lambda} \frac{\partial A}{\partial \beta'_\lambda},$$

$$\frac{\partial^2(A+BC)}{\partial \beta_\mu \partial \beta'_\mu} = C \frac{\partial^2 B}{\partial \beta_\mu \partial \beta'_\mu} (1 - B\delta_{ij}) - \delta_{ij} \frac{\partial B}{\partial \beta_\mu} \left(C \frac{\partial B}{\partial \beta'_\mu} + \frac{\partial AB}{\partial \beta'_\mu} \right),$$

and

$$\frac{\partial^2(A + BC)}{\partial\beta_\lambda\partial\beta'_\mu} = -\delta_{ij} \frac{\partial A}{\partial\beta_\lambda} \left[B \frac{\partial C}{\partial\beta'_\mu} + C \frac{\partial B}{\partial\beta'_\mu} \right].$$

The second derivatives of $(B + AC)$ are

$$\begin{aligned} \frac{\partial^2(B + AC)}{\partial\beta_\lambda\partial\beta'_\lambda} &= C \frac{\partial^2 A}{\partial\beta_\lambda\partial\beta'_\lambda} (1 - A\delta_{ij}) - \delta_{ij} \frac{\partial A}{\partial\beta_\lambda} \left(C \frac{\partial A}{\partial\beta'_\lambda} + \frac{\partial BA}{\partial\beta'_\lambda} \right), \\ \frac{\partial^2(B + AC)}{\partial\beta_\mu\partial\beta'_\mu} &= \frac{\partial^2 B}{\partial\beta_\mu\partial\beta'_\mu} (1 - AC\delta_{ij}) + AC\delta_{ij}^2 \frac{\partial B}{\partial\beta_\mu} \frac{\partial B}{\partial\beta'_\mu}, \end{aligned}$$

and

$$\frac{\partial^2(B + AC)}{\partial\beta_\lambda\partial\beta'_\mu} = \frac{\partial A}{\partial\beta_\lambda} \frac{\partial C}{\partial\beta'_\mu} [1 - A\delta_{ij}].$$

The second derivatives of $(A - AC)$ are

$$\begin{aligned} \frac{\partial^2(A - AC)}{\partial\beta_\lambda\partial\beta'_\lambda} &= \frac{\partial^2 A}{\partial\beta_\lambda\partial\beta'_\lambda} - \frac{\partial^2(B + AC)}{\partial\beta_\lambda\partial\beta'_\lambda}, \\ \frac{\partial^2(A - AC)}{\partial\beta_\mu\partial\beta'_\mu} &= AC\delta_{ij} \left[\frac{\partial^2 B}{\partial\beta_\mu\partial\beta'_\mu} - \delta_{ij} \frac{\partial B}{\partial\beta_\mu} \frac{\partial B}{\partial\beta'_\mu} \right], \end{aligned}$$

and

$$\frac{\partial^2(A - AC)}{\partial\beta_\lambda\partial\beta'_\mu} = -\frac{\partial^2(B + AC)}{\partial\beta_\lambda\partial\beta'_\mu}.$$

The second derivatives of $(B - BC)$ are

$$\begin{aligned} \frac{\partial^2(B - BC)}{\partial\beta_\lambda\partial\beta'_\lambda} &= BC\delta_{ij} \left[\frac{\partial^2 A}{\partial\beta_\lambda\partial\beta'_\lambda} - \delta_{ij} \frac{\partial A}{\partial\beta_\lambda} \frac{\partial A}{\partial\beta'_\lambda} \right], \\ \frac{\partial^2(B - BC)}{\partial\beta_\mu\partial\beta'_\mu} &= \frac{\partial^2 B}{\partial\beta_\mu\partial\beta'_\mu} - \frac{\partial^2(A + BC)}{\partial\beta_\mu\partial\beta'_\mu}, \end{aligned}$$

and

$$\frac{\partial^2(B - BC)}{\partial\beta_\lambda\partial\beta'_\mu} = -\frac{\partial^2(A + BC)}{\partial\beta_\lambda\partial\beta'_\mu}.$$

Additionally,

$$\frac{\partial^2 A}{\partial\beta_\lambda\partial\beta'_\lambda} = A\mathbf{x}_{i,j-1}\mathbf{x}'_{i,j-1}$$

and

$$\frac{\partial^2 B}{\partial\beta_\mu\partial\beta'_\mu} = B\mathbf{x}_{i,j-1}\mathbf{x}'_{i,j-1}.$$

Here, we present the first derivatives necessary to compute the functions above.

The first derivatives of $(A + BC)$ are

$$\frac{\partial(A + BC)}{\partial\beta_\lambda} = \frac{\partial A}{\partial\beta_\lambda} (1 - BC\delta_{ij})$$

and

$$\frac{\partial(A + BC)}{\partial\beta_\mu} = C \frac{\partial B}{\partial\beta_\mu} (1 - B\delta_{ij}).$$

The first derivatives of $(B + AC)$ are

$$\frac{\partial(B + AC)}{\partial\beta_\lambda} = C \frac{\partial A}{\partial\beta_\lambda} (1 - A\delta_{ij})$$

and

$$\frac{\partial(B + AC)}{\partial\beta_\mu} = \frac{\partial B}{\partial\beta_\mu} (1 - AC\delta_{ij}).$$

The first derivatives of $(A - AC)$ are

$$\frac{\partial(A - AC)}{\partial\beta_\lambda} = \frac{\partial A}{\partial\beta_\lambda} - \frac{\partial(B + AC)}{\partial\beta_\lambda}$$

and

$$\frac{\partial(A - AC)}{\partial\beta_\mu} = AC\delta_{ij} \frac{\partial B}{\partial\beta_\mu}.$$

The first derivatives of $(B - BC)$ are

$$\frac{\partial(B - BC)}{\partial\beta_\lambda} = BC\delta_{ij} \frac{\partial A}{\partial\beta_\lambda}$$

and

$$\frac{\partial(B - BC)}{\partial\beta_\mu} = \frac{\partial B}{\partial\beta_\mu} - \frac{\partial(A + BC)}{\partial\beta_\mu}.$$

Additionally,

$$\frac{\partial A}{\partial\beta_\lambda} = A\mathbf{x}_{i,j-1},$$

$$\frac{\partial A}{\partial\beta_\mu} = \mathbf{0},$$

$$\frac{\partial B}{\partial\beta_\lambda} = \mathbf{0},$$

$$\frac{\partial B}{\partial\beta_\mu} = B\mathbf{x}_{i,j-1}$$

$$\frac{\partial C}{\partial \beta_\lambda} = -C \delta_{ij} \frac{\partial A}{\partial \beta_\lambda},$$

and

$$\frac{\partial C}{\partial \beta_\mu} = -C \delta_{ij} \frac{\partial B}{\partial \beta_\mu}.$$

Now, the components of the conditional covariance matrix, $\text{var} \left\{ \frac{\partial \log \pi(\Phi, \gamma | \mathbf{y})}{\partial \Phi} \middle| \hat{\Phi}, \mathbf{y} \right\}$, are defined as:

$$\text{cov} \left[\frac{\partial \log \pi(\Phi, \gamma | \mathbf{y})}{\partial \beta}, \frac{\partial \log \pi(\Phi, \gamma | \mathbf{y})}{\partial \beta} \right] = \text{diag} \left(\hat{\beta}^2 \circ \left[\frac{1}{v_0^2} (1 - \mathbf{p}^*) + \frac{1}{v_1^2} \mathbf{p}^* \right] - \left[\hat{\beta} \circ \left[\frac{1}{v_0} (1 - \mathbf{p}^*) + \frac{1}{v_1} \mathbf{p}^* \right] \right]^2 \right),$$

$$\text{cov} \left[\frac{\partial \log \pi(\Phi, \gamma | \mathbf{y})}{\partial \beta}, \frac{\partial \log \pi(\Phi, \gamma | \mathbf{y})}{\partial \theta} \right] = - \left[\frac{1}{\hat{\theta}} + \frac{1}{1 - \hat{\theta}} \right] \left[\frac{\hat{\beta} \circ \mathbf{p}^*}{v_1} - (\hat{\beta} \circ \mathbf{p}^*) \circ \left[\frac{\mathbf{p}^*}{v_1} + \frac{1 - \mathbf{p}^*}{v_0} \right] \right],$$

and

$$\text{var} \left[\frac{\partial \log \pi(\Phi, \gamma | \mathbf{y})}{\partial \theta} \right] = \left[\frac{1}{\hat{\theta}} + \frac{1}{1 - \hat{\theta}} \right]^2 \text{var} \left[\sum_{r=1}^p \gamma_{\lambda,r} + \gamma_{\mu,r} \right],$$

where $\beta' = (\beta'_\lambda, \beta'_\mu)$ and $\text{var}[\gamma_r] = \hat{\theta}(1 - \hat{\theta})$. Additionally, $\mathbf{p}^{*'} = (\mathbf{p}_{\lambda}^{*'}, \mathbf{p}_{\mu}^{*'})$, $\mathbf{p}_{\lambda}^{*'} = (p_{\lambda,0}^*, \dots, p_{\lambda,p}^*)$, and $\mathbf{p}_{\mu}^{*'} = (p_{\mu,0}^*, \dots, p_{\mu,p}^*)$. Recall that setting $p_{\lambda,0}^* \equiv 1$ and $p_{\mu,0}^* \equiv 1$ forces λ_0 and μ_0 into the model.

Web Appendix D: Data Generation

To evaluate the performance of our method, we apply it to multiple simulated data sets in a variety of research scenarios. In all of the generated data sets, each individual is allowed to transition between smoking, S, and non-smoking, N, states over a period of time. First, each individual is randomly assigned to an initial state following a draw from a Bernoulli distribution with probability 0.50. Since there are two states in this process, an individual always transitions into the opposite state. True transition times follow an exponential distribution that is parametrized with transition rate λ^{ij} if the individual is currently in an N state and μ^{ij} if he/she is in an S state. Here, we set the true transition rates to

$$\lambda^{ij} = \exp(0.5 - 0.5x_{ij1} + 0.5x_{ij2} - 0.5x_{ij5})$$

$$\mu^{ij} = \exp(0.5 + 0.5x_{ij1} + 0.5x_{ij5} - 0.5x_{ij6})$$

We restrict our analysis to weaker effects, under the assumption that performance will only improve with larger effects (Koslovsky et al., 2016). The full model contains 4 binary covariates $(x_{ij1}, \dots, x_{ij4})$ and 16 continuous covariates $(x_{ij5}, \dots, x_{ij20})$. Recall that since covariates can be associated with both transition rates, this creates $2^{2 \times 20} > 10^{12}$ possible models. Binary covariates are sampled from a Bernoulli distribution with probability 0.50. Binary covariates x_{ij1} and x_{ij3} are resampled from the same distribution after the individual has transitioned 10 times. Continuous covariates $(x_{ij6}, x_{ij8}, \dots, x_{ij20})$ follow a multivariate normal distribution with mean 0, variance 1, and an exchangeable correlation structure, $\rho = 0$ or $\rho = 0.75$. Continuous covariates x_{ij5} and x_{ij7} are simulated from a random walk with the initial value sampled from a normal distribution with mean 0 and variance 1. Thereafter, the data are generated by $x_{i,j} = x_{i,j-1} + \epsilon_{i,j}$, where $\epsilon_{i,j}$ is sampled from a normal distribution with mean 0 and variance 0.001 at each transition.

The true transition process is iterated until an individual's cumulative transition time exceeds the period of time for which he/she is set to be followed (e.g., 30 or 70 units of time). In practice, we do not always observe an assessment exactly at each individual's transition time. We only observe their current state at each assessment time. For example, an individual may receive a post-quit random assessment at 8 a.m., slip at 8:05 a.m., and not perform another assessment until 8:20 a.m. Here, the exact transition time is unknown since we only observe N at 8 a.m. and S at 8:20 a.m. To analogue this, we parse through each individual's simulated transition data at equally or randomly spaced assessment times and identify the individual's state at the time the assessment is conducted. At each assessment time, we observe the individual's current smoking state and measured risk factors. Then all of the individuals' observations are compiled to create the data set for analysis.

Web Appendix E: Simulations

Here, we examine the performance of our method in various scenarios. For scenarios 1-8, we simulate $m = 100$ and $m = 150$ individuals observed at $n_i = 30$ or $n_i = 70$ equally spaced assessments under both correlation structures. Equally spaced observations are a special case of a continuous-time Markov process which can be modeled discretely. Thus in these scenarios, we can model the data with a discrete-time transition model, as in (Diggle et al., 2013), for comparison:

$$\text{logit}(\omega_S(\mathbf{x}_{i,j-1}) | y_{i,j-1} = N) = 0.5 - 0.5x_{i,j-1,1} + 0.5x_{i,j-1,2} - 0.5x_{i,j-1,5} \quad (\text{A.3})$$

and

$$\text{logit}(\omega_N(\mathbf{x}_{i,j-1}) | y_{i,j-1} = S) = 0.5 + 0.5x_{i,j-1,1} + 0.5x_{i,j-1,5} - 0.5x_{i,j-1,6} \quad (\text{A.4})$$

where $\omega_S(\mathbf{x}_{i,j-1})$ and $\omega_N(\mathbf{x}_{i,j-1})$ are the probabilities that an individual is observed in a smoking or non-smoking state at t_{ij} , respectively. Note, we use the covariates observed in the current state to model the probability of transition in the next state, similar to Eq. 3 in the main article. Here, we can compare our method to any variable selection method designed for logistic regression models; we choose the LASSO (Tibshirani, 1996) and EMVS (Koslovsky et al., 2016). Note that EMVS for logistic regression models has already been shown to outperform stepwise selection procedures (Koslovsky et al., 2016).

For scenarios 9-16, we simulate $m = 100$ and $m = 150$ individuals observed at $n_i = 30$ or $n_i = 70$ randomly spaced assessments under both correlation structures. Since observation times are inconsistent, this data structure is more realistic for EMA data. Consequently, modeling the data with Eq. A.3 and A.4 for comparison is no longer valid.

Each scenario is simulated 250 times and evaluated in R (R Core Team, 2015). We initialize our method using estimates from the **msm** package (Jackson et al., 2011) for a two-state model including all possible covariates. Before selection, we standardize continuous covariates to mean 0 and variance 1. The sparsity parameter θ is initially set to 0.50. The variance of

exclusion and inclusion are set similar to the method suggested by Koslovsky et al. (2016). Here, we claim a hazard ratio between (0.95, 1.05) to be clinically irrelevant, and we evaluate the local stability of regularization plots around our intuition with a 95% prior probability of inclusion for the hazards ratio that covers (1/4, 4). Using this tuning procedure, we set the 95% prior probability of exclusion equivalent to a hazards ratio between (0.95, 1.05), $v_0 = 0.0006$, for all models. For the comparisons in scenarios 1-8, EMVS for logistic regression models are tuned similarly. We use the **glmnet** package to compare our model with the LASSO for logistic regression (Friedman et al., 2009). Here, each LASSO model is tuned using 10-fold cross validation to identify the largest penalty value, λ_{LASSO} , that is within one standard error of the minimum mean square error (Breiman et al., 1984). For the annealing process, the inverse temperature is initially set to .2 and increased by .1 until $t = 1$, as described in Web Appendix B. Convergence at each temperature level and at each CM-step using the Newton-Raphson algorithm is determined with $\epsilon = 1e - 5$.

To evaluate the performance of our method, we calculate the average false positive (FP) and false negative (FN) rates with $FPR = FP/(FP + TN)$ and $FNR = FN/(FN + TP)$, where TP and TN are true positives and true negatives, respectively. Additionally, we assessed the bias (average of the posterior modes minus true values), the Monte Carlo error of the posterior modes (MCE), the square root of the average of the posterior variances estimated with Louis's method (SE), the coverage probability (CP) of the 95% equal-tail credible intervals, and the average mean squared error (MSE) of the steady-state probability of transition from a non-smoking to a smoking state.

Web Appendix F: Simulation Results

The simulation results for scenarios 1-8 are found in Table 1. Here, our method produced relatively low FPR and FNR. The performance of our method improved with larger sam-

ple sizes and number of assessments observed and declined with higher correlation among covariates.

[Table 1 about here.]

Across all combinations of the number of individuals, number of assessments, and correlation structures, our method correctly included associated covariates in 99.4% of the simulations on average (min = 94.4% and max = 100%). Additionally, our method correctly excluded unassociated covariates in 99.2% of the simulations on average (min = 88.8% and max = 100%). Marginally, we observed that our method performed better for continuous covariates. It was least accurate for binary covariates whose values were allowed to change. With equally spaced assessment times, our method estimated unknown parameters with minimal bias, MCE very close to the SE, and CP around 92% on average (Table 2). The MSE for the steady-state probability of transition from a non-smoking to a smoking state was around 0.04 for scenarios 1-8. In terms of the MSE, our method performed better with higher correlation structures and was insensitive to the number of individuals and number of assessments (Table 3).

[Table 2 about here.]

[Table 3 about here.]

Our method outperformed or showed relatively equivalent performance to the LASSO in FPR and FNR in every setting (Table 1). In sensitivity analyses not shown, we found the LASSO tuned with a λ_{LASSO} that was within one standard error of the minimum performed better than a λ_{LASSO} that minimized the cross-validation error in our simulations. Additionally, the LASSO method was outperformed by EMVS for logistic regression models. EMVS for multistate models on data with equally spaced assessment times showed comparable performance to EMVS for logistic regression models. Here, EMVS for multistate models

performed better in all of the 8 scenarios for average FPR. However, EMVS for logistic regression performed better in 4 of the 8 scenarios for average FNR. The differences in performance were small and could be attributed to tuning parameterization.

In scenarios 9-16, we found the performance of EMVS for multistate models on data with randomly spaced assessment times was marginally worse than that for data with for equally spaced assessment times (Table 4). This discrepancy could be due to smaller observation windows for some individuals, since their first and last assessments may be later or earlier than the equally spaced assessments, respectively.

[Table 4 about here.]

Across all combinations of the number of individuals, number of assessments, and correlation structures, the method correctly selected associated covariates in 98.7% of the simulations on average (min = 93.2% and max = 100%). Additionally, the method correctly excluded unassociated covariates in 98.7% of the simulations on average (min 87.6% and max 100%). Again, the method performed better for continuous covariates than binary covariates. With randomly spaced assessment times, our method estimated unknown parameters with minimal bias, MCE very close to the SE, and CP around 92% on average, similar to the results found with equally spaced assessment times (Table 5). Additionally, the MSE for the steady-state probability of transition from a non-smoking state to a smoking state with randomly spaced assessments was similar to the MSE observed with the equally spaced assessments (Table 3).

[Table 5 about here.]

[Figure 1 about here.]

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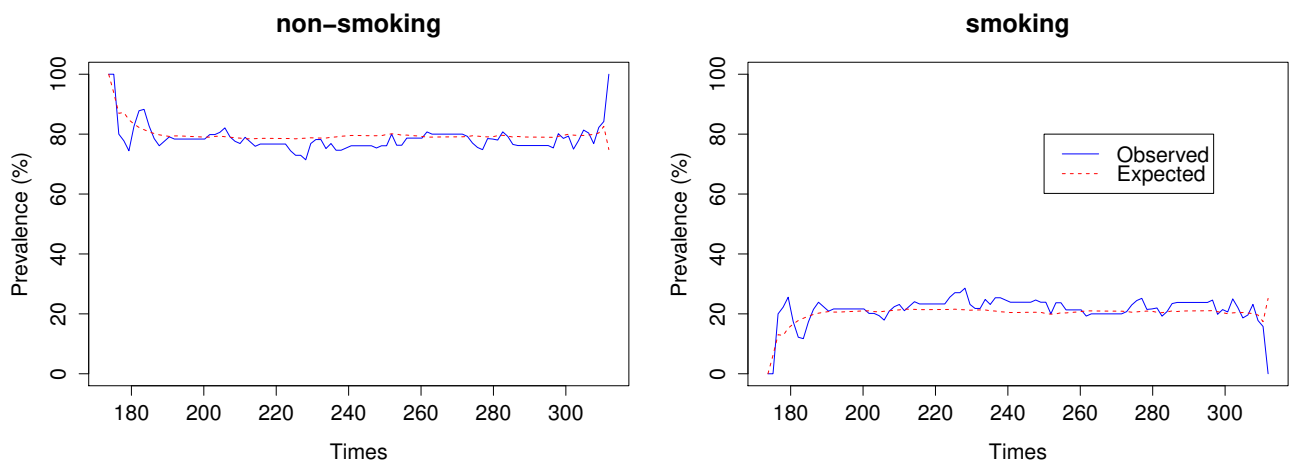


Figure 1. Estimated and observed smoking and non-smoking prevalence one week after the quit attempt in the PREVAIL Study. Time is in days.

Table 1

*Simulation Scenarios 1-8 Results: Comparison of selection performance between EMVS for multistate models and the LASSO and EMVS for logistic regression models when assessment times are equally spaced. The number of **Individuals**, number of **Assessments**, and correlation structure between covariates, ρ , is varied in each scenario. Here, the false positive (**FPR**) and false negative (**FNR**) rates are compared.*

Individuals	Assessments	ρ	FPR			FNR		
			a	b	c	a	b	c
100	30	0	0.010	-0.026	-0.011	0.017	0.017	-0.023
100	30	0.75	0.030	-0.038	0.005	0.020	0.019	-0.056
100	70	0	0.002	-0.037	-0.028	0.000	0.000	-0.002
100	70	0.75	0.002	-0.030	-0.026	0.000	0.000	-0.001
150	30	0	0.004	-0.031	-0.017	0.002	0.002	-0.013
150	30	0.75	0.011	-0.036	-0.014	0.003	0.003	-0.019
150	70	0	0.000	-0.041	-0.031	0.000	0.000	0.000
150	70	0.75	0.000	-0.029	-0.021	0.000	0.000	-0.001

^a EMVS for multistate models

^b EMVS for multistate models - EMVS for logistic models

^c EMVS for multistate models - LASSO

Table 2

Simulation Scenarios 1-8 Results: Evaluation of Bias and Monte Carlo Error (MCE) of the estimated, unknown parameters, square root of the average Louis's method posterior variance estimates (SE), and coverage probabilities (CP) of equal tailed 95% credible intervals at varying numbers of individuals, assessments, and correlation structures, ρ , for equally spaced assessment times.

	True Effect	100 Individuals				150 Individuals			
		Bias	MCE	SE	CP	Bias	MCE	SE	CP
30 Assessments $\rho = 0$	λ_0	0.029	0.127	0.108	0.900	0.022	0.091	0.088	0.928
	$\beta_{\lambda,1}$	0.024	0.159	0.127	0.908	0.009	0.109	0.106	0.956
	$\beta_{\lambda,2}$	-0.026	0.134	0.108	0.932	-0.010	0.085	0.088	0.960
	$\beta_{\lambda,5}$	0.004	0.090	0.078	0.932	-0.003	0.068	0.064	0.940
	μ_0	0.056	0.127	0.097	0.856	0.037	0.093	0.078	0.884
	$\beta_{\mu,1}$	-0.021	0.151	0.127	0.916	-0.025	0.104	0.106	0.956
	$\beta_{\mu,5}$	0.000	0.092	0.078	0.928	0.000	0.070	0.064	0.916
30 Assessments $\rho = 0.75$	$\beta_{\mu,6}$	0.002	0.073	0.059	0.896	0.002	0.057	0.048	0.912
	λ_0	0.042	0.126	0.102	0.868	0.029	0.097	0.083	0.900
	$\beta_{\lambda,1}$	-0.001	0.144	0.122	0.940	0.003	0.105	0.100	0.956
	$\beta_{\lambda,2}$	-0.017	0.138	0.101	0.916	-0.011	0.095	0.084	0.928
	$\beta_{\lambda,5}$	0.000	0.130	0.094	0.908	-0.001	0.089	0.079	0.920
	μ_0	0.050	0.106	0.091	0.880	0.039	0.086	0.074	0.904
	$\beta_{\mu,1}$	-0.023	0.149	0.121	0.940	-0.018	0.113	0.100	0.928
70 Assessments $\rho = 0$	$\beta_{\mu,5}$	-0.015	0.143	0.101	0.876	-0.006	0.088	0.083	0.956
	$\beta_{\mu,6}$	0.018	0.119	0.087	0.888	0.005	0.080	0.072	0.940
	λ_0	0.013	0.083	0.071	0.896	0.010	0.066	0.058	0.904
	$\beta_{\lambda,1}$	-0.003	0.085	0.086	0.972	0.002	0.066	0.070	0.960
	$\beta_{\lambda,2}$	-0.006	0.072	0.072	0.944	-0.007	0.057	0.058	0.956
	$\beta_{\lambda,5}$	0.000	0.062	0.051	0.904	-0.001	0.051	0.042	0.892
	μ_0	0.023	0.098	0.063	0.772	0.010	0.081	0.052	0.784
70 Assessments $\rho = 0.75$	$\beta_{\mu,1}$	-0.016	0.088	0.086	0.928	-0.008	0.069	0.070	0.940
	$\beta_{\mu,5}$	-0.001	0.064	0.051	0.892	0.003	0.049	0.042	0.900
	$\beta_{\mu,6}$	0.004	0.050	0.039	0.860	0.004	0.040	0.033	0.868
	λ_0	0.002	0.080	0.067	0.900	-0.001	0.071	0.055	0.896
	$\beta_{\lambda,1}$	0.002	0.072	0.081	0.976	0.007	0.062	0.066	0.960
	$\beta_{\lambda,2}$	-0.005	0.064	0.067	0.960	-0.004	0.056	0.055	0.940
	$\beta_{\lambda,5}$	-0.005	0.072	0.065	0.936	0.002	0.060	0.056	0.920
μ_0	0.018	0.067	0.060	0.916	0.014	0.054	0.050	0.928	
$\beta_{\mu,1}$	-0.017	0.077	0.080	0.952	-0.011	0.063	0.065	0.948	
$\beta_{\mu,5}$	-0.002	0.076	0.068	0.928	0.006	0.064	0.057	0.924	
$\beta_{\mu,6}$	0.003	0.073	0.060	0.880	0.000	0.062	0.050	0.896	

Table 3

Simulation scenarios 1-16: Evaluation of the steady-state probability MSE at varying numbers of individuals, assessments, and correlation structures, ρ , for equal spaced and randomly spaced assessment times.

Individuals	Assessments	ρ	Equally Spaced	Randomly Spaced
100	30	0	0.0581	0.0583
100	30	0.75	0.0349	0.0345
100	70	0	0.0586	0.0590
100	70	0.75	0.0348	0.0352
150	30	0	0.0583	0.0575
150	30	0.75	0.0347	0.0345
150	70	0	0.0582	0.0583
150	70	0.75	0.0347	0.0349

Table 4

*Simulation Scenarios 9-16 Results: Selection performance using EMVS for multistate models when assessment times are randomly spaced. The number of **Individuals**, number of **Assessments**, and correlation structure between covariates, ρ , is varied in each scenario. Here, the false positive (**FPR**) and false negative (**FNR**) rates are presented.*

Individuals	Assessments	ρ	FPR	FNR
100	30	0	0.016	0.024
100	30	0.75	0.049	0.039
100	70	0	0.003	0.001
100	70	0.75	0.005	0.001
150	30	0	0.007	0.010
150	30	0.75	0.017	0.010
150	70	0	0.001	0.000
150	70	0.75	0.001	0.000

Table 5

Simulation Scenarios 9-16 Results: Evaluation of Bias and Monte Carlo error (MCE) of the estimated, unknown parameters, square root of the average Louis's method posterior variance estimates (SE), and coverage probabilities (CP) of equal tailed 95% credible intervals at varying numbers of individuals, assessments, and correlation structures, ρ , for randomly spaced assessment times.

	True Effect	100 Individuals				150 Individuals			
		Bias	MCE	SE	CP	Bias	MCE	SE	CP
30 Assessments $\rho = 0$	λ_0	0.008	0.153	0.121	0.860	-0.025	0.112	0.099	0.892
	$\beta_{\lambda,1}$	-0.008	0.157	0.141	0.916	0.004	0.129	0.118	0.936
	$\beta_{\lambda,2}$	-0.052	0.154	0.119	0.908	-0.035	0.116	0.098	0.936
	$\beta_{\lambda,5}$	0.005	0.103	0.085	0.904	0.003	0.076	0.070	0.944
	μ_0	0.000	0.146	0.108	0.844	-0.019	0.118	0.088	0.856
	$\beta_{\mu,1}$	-0.071	0.173	0.140	0.896	-0.059	0.144	0.117	0.924
	$\beta_{\mu,5}$	0.001	0.103	0.086	0.896	-0.003	0.077	0.070	0.912
30 Assessments $\rho = 0.75$	λ_0	0.007	0.082	0.064	0.896	0.008	0.063	0.052	0.896
	λ_0	-0.031	0.150	0.114	0.868	-0.044	0.116	0.094	0.872
	$\beta_{\lambda,1}$	0.020	0.182	0.134	0.892	0.019	0.128	0.112	0.948
	$\beta_{\lambda,2}$	-0.037	0.141	0.114	0.936	-0.028	0.112	0.093	0.920
	$\beta_{\lambda,5}$	0.015	0.169	0.103	0.860	-0.002	0.101	0.086	0.916
	μ_0	-0.016	0.120	0.102	0.896	-0.024	0.095	0.083	0.908
	$\beta_{\mu,1}$	-0.046	0.166	0.133	0.908	-0.039	0.121	0.112	0.940
70 Assessments $\rho = 0$	$\beta_{\mu,5}$	-0.016	0.168	0.111	0.864	-0.010	0.105	0.092	0.924
	$\beta_{\mu,6}$	0.033	0.143	0.098	0.888	0.018	0.092	0.080	0.940
	λ_0	-0.001	0.094	0.081	0.924	-0.013	0.079	0.067	0.904
	$\beta_{\lambda,1}$	-0.002	0.093	0.098	0.952	-0.002	0.074	0.080	0.964
	$\beta_{\lambda,2}$	-0.009	0.091	0.081	0.940	-0.006	0.068	0.066	0.920
	$\beta_{\lambda,5}$	0.000	0.065	0.057	0.896	0.000	0.052	0.046	0.916
	μ_0	-0.001	0.100	0.072	0.860	-0.006	0.082	0.059	0.836
70 Assessments $\rho = 0.75$	$\beta_{\mu,1}$	-0.033	0.096	0.097	0.948	-0.028	0.078	0.080	0.952
	$\beta_{\mu,5}$	0.000	0.067	0.057	0.888	0.002	0.053	0.047	0.912
	$\beta_{\mu,6}$	0.000	0.055	0.043	0.888	0.000	0.046	0.036	0.856
	λ_0	-0.020	0.088	0.077	0.896	-0.025	0.076	0.063	0.872
	$\beta_{\lambda,1}$	0.013	0.084	0.092	0.940	0.009	0.076	0.075	0.924
	$\beta_{\lambda,2}$	-0.006	0.073	0.076	0.964	-0.002	0.060	0.062	0.964
	$\beta_{\lambda,5}$	-0.001	0.075	0.072	0.940	-0.002	0.066	0.061	0.936
μ_0	-0.013	0.076	0.068	0.920	-0.012	0.061	0.056	0.932	
$\beta_{\mu,1}$	-0.014	0.088	0.092	0.948	-0.012	0.069	0.075	0.964	
$\beta_{\mu,5}$	-0.003	0.079	0.076	0.936	0.002	0.062	0.064	0.960	
$\beta_{\mu,6}$	0.011	0.077	0.066	0.932	0.007	0.056	0.055	0.928	