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ASSESSING TIME-VARYING CAUSAL EFFECT MODERATION IN THE PRESENCE OF CLUSTER-LEVEL TREATMENT EFFECT HETEROGENEITY AND INTERFERENCE

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Abstract

The micro-randomized trial (MRT) is a sequential randomized experimental design to empirically evaluate the effectiveness of mobile health (mHealth) intervention components that may be delivered at hundreds or thousands of decision points. MRTs have motivated a new class of causal estimands, termed “causal excursion effects”, for which semiparametric inference can be conducted via a weighted, centered least squares criterion (Boruvka et al., 2018). Existing methods assume between-subject independence and non-interference. Deviations from these assumptions often occur. In this paper, causal excursion effects are revisited under potential cluster-level treatment effect heterogeneity and interference, where the treatment effect of interest may depend on cluster-level moderators. Utility of the proposed methods is shown by analyzing data from a multi-institution cohort of first year medical residents in the United States.

Keywords

Causal Inference; Clustered Data; Just-In-Time Adaptive Interventions; Microrandomized Trials; Mobile Health; Moderation Effect

1. INTRODUCTION

Modern behavioral science has placed a considerable amount of attention on push notifications sent via mobile device that are adapted to continuously collected information on an individual’s current context. These time-varying adaptive interventions are hypothesized to lead to meaningful short- and long-term behavior change. The assessment of the time-varying effect of such push notifications motivated sequential randomized designs such as the micro-randomized trial (MRT) [1, 2], in which individuals are randomized to potentially receive notifications at hundreds or thousands of decision points. The MRT design enables the estimation of marginal treatment effects of push notifications on prespecified time-lagged outcomes of interest, referred to as “causal excursion effects” [3,

4, 5]. Semiparametric inference of the causal excursion effects can be conducted via a weighted, centered least squares (WCLS) criterion [3].

The WCLS inferential method relies on two key assumptions. First, an intervention delivered to an individual is assumed to only impact that same individual's outcomes, i.e., between-subject non-interference. Second, the method assumes no stochastic dependence among outcomes of different subjects. Deviations from these assumptions, however, may occur when individuals naturally form clusters. To address these violations, this paper extends the definition of causal excursion effects to account for potential interference and cluster-level treatment effect heterogeneity accompanied with a general inferential approach that provides valid inferences and subsumes WCLS as a special case.

2. PRELIMINARIES

2.1. Micro-Randomized Trials (MRT).

An MRT consists of a sequence of within-subject decision times $t = 1, \dots, T$ at which treatment options may be randomly assigned [6]. Individual-level data can be summarized as $\{O_0, O_1, A_1, O_2, A_2, \dots, O_T, A_T, O_{T+1}\}$ where t indexes a sequence of decision points, O_0 is the baseline information, O_t is the information collected between time $t - 1$ and t , and A_t is the treatment option provided at time t ; for simplicity, we consider binary treatment options, i.e., $A_t \in \{0, 1\}$. In an MRT, A_t is randomized according to a known sequence of randomization probabilities that may depend on the complete observed history $H_t := \{O_0, O_1, A_1, \dots, A_{t-1}, O_t\}$, denoted $\mathbf{p} = \{p_t(A_u | H_u)\}_{u=1}^t$. Treatment options are designed to impact a proximal response, denoted by $Y_{t,\Delta}$, which is a known function of the participant's data within a subsequent window of length $\Delta \geq 1$, i.e., $Y_{t,\Delta} = y(O_t, A_t, O_{t+1}, A_{t+1}, \dots, A_{t+\Delta-1}, O_{t+\Delta})$ [5].

2.2 Estimand and Inferential Method: A Review.

We focus on the class of estimands referred to as “causal excursion effects”, which are time-varying as a function of the decision point t . We provide formal definitions using potential outcomes [7, 8]. Let $Y_{t,\Delta}(\bar{a}_{t+\Delta-1})$ denote the potential outcome for the proximal response under treatment sequence $\bar{a}_{t+\Delta-1} = (a_1, \dots, a_{t+\Delta-1})$. Let $S_t(\bar{a}_{t-1})$ denote the potential outcome for a potential time-varying effect moderator which is a deterministic function of the potential history up to time t , $H_t(\bar{a}_{t-1})$. The causal excursion effect is then defined with respect to a *reference distribution*, i.e., the distribution of treatments $\bar{A}_{t+\Delta-1} := \{A_1, \dots, A_{t+\Delta-1}\}$. For past treatments, \bar{A}_t , we follow common practice in observational mobile health studies where analyses such as GEEs [9] are conducted marginally over the distribution of historical information. A similar strategy here is to use the past treatment randomization probabilities as the reference distribution between time 1 and t . For future treatments, the choice of distribution for $\tilde{A}_{t+1:(t+\Delta-1)} := (A_{t+1}, \dots, A_{t+\Delta-1})$ may differ by the type of inference desired; note that when $\Delta = 1$, future treatments do not impact the proximal outcome and therefore a reference distribution for future treatments is not necessary. Here, we assume the reference distribution for treatment assignments from $t + 1$ to $t + \Delta - 1$ is given by a randomization probability generically represented by $\pi_u(a_u | H_u)$, $u = t + 1, \dots, t + \Delta - 1$ and let $\pi = \{\pi_u\}_{u=t+1}^{t+\Delta-1}$. This generalization contains previous definitions such as lagged effects [3] where $\pi_u = p_u$

and deterministic choices such as $a_{t+1:(t+\Delta-1)} = \mathbf{0}$ [5, 4] where $\pi_u = \mathbf{1}\{a_u = 0\}$ and $\mathbf{1}\{\bullet\}$ is the indicator function. Then the causal excursion effect $\beta_{p,\pi,\Delta}(t; s)$ is defined as

$$\mathbb{E}_{p,\pi}[Y_{t,\Delta}(\bar{A}_{t-1}, \mathbf{1}, \tilde{A}_{t+1:(t+\Delta-1)}) - Y_{t,\Delta}(\bar{A}_{t-1}, \mathbf{0}, \tilde{A}_{t+1:(t+\Delta-1)}) \mid S_t(\bar{A}_{t-1}) = s] \quad (1)$$

$$= \mathbb{E}_p[\mathbb{E}_p[W_{t,\Delta}Y_{t,\Delta} \mid A_t = 1, H_t] - \mathbb{E}_p[W_{t,\Delta}Y_{t,\Delta} \mid A_t = 0, H_t] \mid S_t = s] \quad (2)$$

where treatment sequence up to time $t-1$: $\bar{A}_{t-1} \sim \mathbf{p}$, future treatment sequence up to $t+\Delta-1$: $\tilde{A}_{t+1:(t+\Delta-1)} \sim \pi$ and $W_{t,\Delta} = \prod_{u=t+1}^{t+\Delta-1} \pi_u(A_u \mid H_u) / p_u(A_u \mid H_u)$ can be interpreted as change of measure from \mathbf{p} to π for treatment assignments $\tilde{A}_{t+1:(t+\Delta-1)}$; we set $W_{t,\Delta} = 1$ when $\Delta = 1$. Equation (2) expresses (1) in terms of observable data, which requires the standard causal inference assumptions of positivity, sequential ignorability, and consistency. Assuming $\beta_{p,\pi,\Delta}(t; s) = f_t(s)^\top \beta^*$ where $f_t(s) \in \mathbb{R}^q$ is a feature vector comprised of a q -dimensional summary of observed state information depending only on state s and decision point t , a consistent estimator for β^* can be obtained by minimizing a weighted and centered least squares (WCLS) criterion:

$$\hat{\beta} = \underset{\alpha, \beta}{\operatorname{argmin}} \mathbb{P}_n \left[\sum_{t=1}^T W_t \times W_{t,\Delta} [Y_{t,\Delta} - g_t(H_t)^\top \alpha - (A_t - \tilde{p}_t(1 \mid S_t)) f_t(S_t)^\top \beta]^2 \right] \quad (3)$$

where \mathbb{P}_n is shorthand for the sample average, $W_t = \tilde{p}_t(A_t \mid S_t) / p_t(A_t \mid H_t)$ is a weight where the numerator is an arbitrary function with range (0, 1) that only depends on potential moderators of interest S_t , and $g_t(H_t) \in \mathbb{R}^p$ are p control variables chosen to help reduce variance and to construct more powerful test statistics. See [3] for more details on the seminal estimand formulation and consistency, asymptotic normality, and robustness properties of the WCLS estimation method.

2.3. Motivating Example.

The Intern Health Study (IHS) is a 6-month MRT on 1,562 medical interns [10]. Due to high depression rates and levels of stress during the first year of physician residency training, a critical question is whether targeted notifications can improve mood, increase sleep time, and/or increase physical activity. Enrolled medical interns were randomized weekly to receive either mood, activity, or sleep notifications or receive no notifications for that week (probability 1/4 each). Analyses conducted in this paper focus on the weekly randomization; see [10] for further study details. Figure 1 presents specialty-specific effect estimates on weekly average mood scores using (3), with evident specialty-level treatment effect heterogeneity. This suggests a marginal analysis must account for effect heterogeneity at the specialty-level. The present work offers such a framework to address the inferential deficiency that we show if the standard WCLS were used under cluster-level effect heterogeneity. In addition, there exists potential within-cluster interference of other subjects' treatments upon a subject's outcome. Our framework defines a new and useful indirect excursion effect under sequential treatments in contrast to existing work that mostly focuses on indirect effects in non-temporal settings.

3. CLUSTER-LEVEL PROXIMAL TREATMENT EFFECTS

3.1. Proximal Moderated Treatment Effects: A Cluster-based Conceptualization.

Consider a cluster of size G . Overbar will continue to denote treatment sequences; $\bar{a}_{t,j} = (a_{1,j}, \dots, a_{t,j})$, for instance, denotes the sequence of realized treatment sequence up to and including decision time t for individual $j \in [G] = \{1, \dots, G\}$. Let $\bar{a}_t = (\bar{a}_{t,1}, \dots, \bar{a}_{t,G})$ denote the set of realized treatments for all individuals in the cluster. Let $\bar{a}_{t,-j} = \bar{a}_t \setminus \bar{a}_{t,j}$ denote this set with the j th individual removed. Let $Y_{t,\Delta,j}(\bar{a}_{t+\Delta-1})$ denote the potential outcome for individual $j \in [G]$ which may depend on realized treatments for all subjects in the cluster.

Direct causal excursion effects.—In standard MRTs, the individual is the unit of interest. Here, the cluster is the unit of interest and the effect of interest is in providing treatment versus not providing treatment at time t on a random individual in the group. This can be expressed as a difference in potential outcomes for the proximal response

$$\frac{1}{G} \sum_{j=1}^G [Y_{t,\Delta,j}(\bar{a}_{t+\Delta-1,-j}, (\bar{a}_{t-1,j}, 1, a_{t+1:(t+\Delta-1),j})) - Y_{t,\Delta,j}(\bar{a}_{t+\Delta-1,-j}, (\bar{a}_{t-1,j}, 0, a_{t+1:(t+\Delta-1),j}))]. \quad (4)$$

Following [11] and [12], (4) is a *group average direct causal effect* of treatment versus no treatment fixing all other treatments.

The “fundamental problem of causal inference” [7, 13] is that individual differences cannot be observed. Thus, similar to prior work [5, 3], averages of potential outcomes are considered. Let $S_t(\bar{a}_{t-1})$ denote a vector of potential moderator variables formed from $H_t(\bar{a}_{t-1})$, the *cluster-level* history up to decision point t . Then the moderated direct treatment effect, denoted $\beta_{p,\pi,\Delta}(t; s)$, can be defined as

$$\mathbb{E}_{p,\pi} [Y_{t,\Delta,J}(\bar{A}_{t+\Delta-1,-J}, (\bar{A}_{t-1,J}, 1, \tilde{A}_{t+1:(t+\Delta-1),J})) - Y_{t,\Delta,J}(\bar{A}_{t+\Delta-1,-J}, (\bar{A}_{t-1,J}, 0, \tilde{A}_{t+1:(t+\Delta-1),J})) \mid S_t(\bar{A}_{t-1}) = s]. \quad (5)$$

where J is a uniformly distributed random index defined on $[G]$. The expectation is over the potential outcomes $Y_{t,\Delta,J}(\cdot)$, the randomized treatments $-\bar{A}_{t+\Delta-1,-J} \sim \mathbf{p}$, $\bar{A}_{t-1,J} \sim \mathbf{p}$, and $\tilde{A}_{t+1:(t+\Delta-1),J} \sim \pi$ —and the random index J . Choice of $S_t(\bar{A}_{t-1})$ depends on the scientific question of interest. A primary analysis may focus on marginal effects and set $S_t(\bar{A}_{t-1}) = \emptyset$. A second analysis may focus on assessing the effect conditional on variables only related to the individual indexed by J and set $S_t(\bar{A}_{t-1}) = X_{t,J}(\bar{A}_{t-1,J})$, i.e., a potential individual-level moderator of interest where $X_{t,J}(\bar{A}_{t-1,J})$ produces a vector of summary variables from the history of individual J , $H_{t,J}(\bar{A}_{t-1,J})$. A third analysis may consider group-level moderators such as $S_t(\bar{A}_{t-1}) = G^{-1} \sum_j X_{t,j}(\bar{A}_{t-1,j})$ or $S_t(\bar{A}_{t-1}) = (X_{t,J}(\bar{A}_{t-1,J}), \frac{1}{G-1} \sum_{j' \neq J} X_{t,j'}(\bar{A}_{t-1,j'}))$. Equation (5) generalizes the *population average direct causal effect* from [12] to a *group-level causal excursion effect* that allows for moderation and time-varying treatments.

Pairwise indirect causal excursion effects.—Of secondary interest is the indirect effect of providing treatment versus not providing treatment to the j th individual at time t on a different individual's proximal response, i.e., pairwise within-cluster treatment interference.

Here, we define the *pairwise indirect causal excursion effect* as

$$\frac{1}{G \cdot (G - 1)} \sum_{j' \neq j} [Y_{t,\Delta,j}(\bar{a}_{t+\Delta-1,-\{j,j'\}}, (\bar{a}_{t-1,j}, 0, a_{t+1:(t+\Delta-1),j}), (\bar{a}_{t-1,j'}, 1, a_{t+1:(t+\Delta-1),j'})) - Y_{t,\Delta,j}(\bar{a}_{t+\Delta-1,-\{j,j'\}}, (\bar{a}_{t-1,j}, 0, a_{t+1:(t+\Delta-1),j}), (\bar{a}_{t-1,j'}, 0, a_{t+1:(t+\Delta-1),j'}))].$$

Again, since individual differences cannot be observed, averages of potential outcomes are considered. The moderated pairwise indirect treatment effect, denoted $\beta_{p,\pi,\Delta}^{(IE)}(t; s)$, is

$$\mathbb{E}_{\mathbf{p},\pi} [Y_{t,\Delta,j}(\bar{A}_{t+\Delta-1,-\{J,J'\}}, (\bar{A}_{t-1,J}, 0, \tilde{A}_{t+1:(t+\Delta-1),J}), (\bar{A}_{t-1,J'}, 1, \tilde{A}_{t+1:(t+\Delta-1),J'})) - Y_{t,\Delta,j}(\bar{A}_{t+\Delta-1,-\{J,J'\}}, (\bar{A}_{t-1,J}, 0, \tilde{A}_{t+1:(t+\Delta-1),J}), (\bar{A}_{t-1,J'}, 0, \tilde{A}_{t+1:(t+\Delta-1),J'}) \mid S_t(\bar{A}_{t-1}) = s]. \tag{6}$$

where J' is uniformly distributed random index on the set $[G] \setminus \{J\}$. The expectation is over both the potential outcomes $Y_{t,\Delta,j}(\cdot)$, randomized treatments $-\bar{A}_{t+\Delta-1,-\{J,J'\}} \sim \mathbf{p}$, $\bar{A}_{t-1,J} \sim \mathbf{p}$, $\bar{A}_{t-1,J'} \sim \mathbf{p}$, $\tilde{A}_{t+1:(t+\Delta-1),J} \sim \pi$, and $\tilde{A}_{t+1:(t+\Delta-1),J'} \sim \pi$ – and the random indices (J and J'). The potential moderator can be written as $S_t(\bar{A}_{t-1}) = (S_{t,J}(\bar{A}_{t-1}), S_{t,J'}(\bar{A}_{t-1}), S_{t,-\{J,J'\}}(\bar{A}_{t-1}))$ to clarify that the variables can contain both information on the two selected individuals as well as others in the cluster. Another pairwise indirect effect can be defined when individual J receives treatment, i.e., $A_{t,J} = 1$ instead of $A_{t,J} = 0$ as in (6).

Remark 3.1.—*The effect defined by (6) generalizes the group average indirect causal effect from [12] to a group-level pairwise indirect causal excursion effect that allows for moderation and time-varying treatments. To see this, note that the excursion effect at each decision time t averages over a particular reference distribution over the past and future treatments up to and including time $t + \Delta - 1$ defined by the MRT randomization probabilities \mathbf{p} and the alternative probability distribution π . The contrast is over two treatment allocations, both where a random individual does not receive treatment, but where in one allocation another random individual receives treatment and in the other allocation that same individual does not receive treatment. [12] consider contrasts between any two randomized treatment allocations conditional on a random individual not receiving treatment in a non-temporal setting. Therefore, per decision time our definition is a special case of their indirect effect where, for a random non-treated individual, we focus on treating or not treating another random individual and marginalizing over all others in the group. More complex contrasts could be derived such as three- or four-way indirect effects; however, the number of combinations grows quickly making estimation unrealistic in our setting. Our choice of contrast was thus motivated by finding an estimand of scientific interest which could be reasonably estimated within the MRT setting, bridging the literature on causal excursions and indirect effects.*

3.2. Causal Excursion Effect Estimand Depends on Treatment Distribution.

Estimands considered here are most similar to average outcomes under a particular dynamic treatment regime $E_{\mu}[Y(A_1, \dots, A_T)]$ where μ denotes the dynamic treatment regime from which the treatments are drawn [14]. Indeed, for any $A_{u,j}$ not contained in $S_t(\bar{A}_{t-1})$, the direct and indirect effects depend on the distribution of $\{A_{u,j}\}_{u \leq t+\Delta-1, j \in [G]}$. Estimands (5) and (6) marginalize over treatments not contained in $S_t(\bar{A}_{t-1})$. Marginalization over different probabilistic assignment of treatments may yield different results. Therefore, the direct and indirect excursion effects depend on the study protocol and choice of alternative distribution π . The reason for this is that micro-randomization is meant to gather information on how to optimize the design of intervention components [15]. The marginal formulation of main and moderation effects contrasts excursions from the current treatment protocol, and mimics analyses used in a factorial design that marginalize over factors including time. See [4, Section 8] for additional considerations. Regardless, the effects considered in this paper are causal and depend on the treatment assignment distributions. Due to this dependence, in real data analysis, we recommend presenting the micro-randomization distribution together with the estimated treatment effects, thus the subscript $(\mathbf{p}, \boldsymbol{\pi})$ in the definition of both the direct and indirect effects are specified.

3.3. Identification.

Causal effects (5) and (6) can be expressed in terms of the observable data under the following standard set of causal inference assumptions [8]:

Assumption 3.2.—We assume consistency, positivity, and sequential ignorability:

- Consistency: For each $t \leq T$ and $j \in [G]$, $\{Y_{t,\Delta,j}(\bar{A}_{t+\Delta-1}), O_{t,j}(\bar{A}_{t-1}), A_{t,j}(\bar{A}_{t-1})\} = \{Y_{t,\Delta,j}, O_{t,j}, A_{t,j}\}$, i.e., observed values equal the corresponding potential outcomes;
- Positivity: if the joint density $\{A_t = a_t, H_t = h_t\}$ is greater than zero, then $P(A_t = a_t | H_t = h_t) > 0$;
- Sequential ignorability: for each $t \leq T$, the potential outcomes, $\{Y_{2,\Delta,j}(\bar{a}_{1+\Delta-1}), O_{2,j}(a_1), A_{2,j}(a_1), \dots, Y_{T,\Delta,j}(\bar{a}_{T+\Delta-1})\}_{j \in [G], \bar{a}_{T+\Delta-1} \in \{0,1\}^{(T+\Delta-1) \times G}}$, are independent of $A_{t,j}$ conditional on the observed history H_t .

Sequential ignorability and, assuming all of the randomization probabilities are bounded away from 0 and 1, positivity, are guaranteed in our setting by design. Consistency is a necessary assumption for linking the potential outcomes as defined here to the data. Since an individual's outcomes may be influenced by the treatments provided to other individuals in the same cluster, consistency holds due to our use of a cluster-based conceptualization of potential outcomes as seen in [16] and [17].

Lemma 3.3.—Under Assumption 3.2, the moderated direct treatment effect $\beta_{\mathbf{p}, \boldsymbol{\pi}, \Delta}(t; s)$ is equal to

$$\mathbb{E}[\mathbb{E}[W_{t,\Delta,j} Y_{t,\Delta,j} | H_t, A_{t,j} = 1] - \mathbb{E}[W_{t,\Delta,j} Y_{t,\Delta,j} | H_t, A_{t,j} = 0] | S_t = s],$$

where expectations are with respect to the distribution of the data collected under the actual treatment assignment probabilities \mathbf{p} , and $W_{t,\Delta,j} = \prod_{u=t+1}^{t+\Delta-1} \pi(A_{u,j} | H_u) / p(A_{u,j} | H_u)$ with $W_{t,1,j} = 1$; and the moderated indirect treatment effect $\beta_{\mathbf{p},\pi,\Delta}^{(IE)}(t; s)$ is equal to

$$\begin{aligned} & \mathbb{E}[\mathbb{E}[W_{t,\Delta,j,j} Y_{t,\Delta,j} | H_t, A_{t,j} = 0, A_{t,j'} = 1]] \\ & - \mathbb{E}[W_{t,\Delta,j,j} Y_{t,\Delta,j} | H_t, A_{t,j} = 0, A_{t,j'} = 0] | S_t = s]. \end{aligned}$$

where $W_{t,\Delta,j,j'} = \prod_{u=t+1}^{t+\Delta-1} \pi_u(A_{u,j}, A_{u,j'} | H_u) / p_u(A_{u,j}, A_{u,j'} | H_u)$ with $W_{t,1,j,j'} = 1$.

Proof of Lemma 3.3 can be found in the Appendix A.

4. ESTIMATION

4.1. Direct Causal Excursion Effect Estimation.

Assumption 4.1.—Assume the direct causal excursion effect $\beta_{\mathbf{p},\pi,\Delta}(t; s) = f_t(s)^\top \beta^*$ where $f_t(s) \in \mathbb{R}^q$ is a q -dimensional feature vector that is a function of moderator state s and decision point t .

Consider inference on the q -dimensional parameter β^* . Define the weight $W_{t,j}$ at deci $\frac{\tilde{p}_t(A_{t,j} | S_t)}{p(A_{t,j} | H_t)}$ where $\tilde{p}_t(a | S_t) \in (0, 1)$ is arbitrary as long as it does not depend on terms in H_t other than S_t , and $p(A_{t,j} | H_t)$ is the marginal probability that individual j receives treatment $A_{t,j}$ given H_t . Here we consider an estimator which is the minimizer of a cluster-based, weighted-centered least-squares (C-WCLS) criterion:

$$\mathbb{P}_M \left[\frac{1}{G_m} \sum_{j=1}^{G_m} \sum_{t=1}^T W_{t,j} \times W_{t,\Delta,j} (Y_{t,\Delta,j} - g_t(H_t)^\top \alpha - (A_{t,j} - \tilde{p}_t(A_{t,j} | S_t)) f_t(S_t)^\top \beta)^2 \right] \quad (7)$$

where \mathbb{P}_M is defined as the average of a function over the sample, which in this context is the sample of *clusters* rather than the sample of *individuals* as in traditional MRT settings. In Appendix B, we prove the following result.

Lemma 4.2.—Under Assumption 4.1, given invertibility and moment conditions, the estimator $\hat{\beta}$ that minimizes (7) satisfies $\sqrt{M}(\hat{\beta} - \beta^*) \rightarrow N(0, Q^{-1} W Q^{-1})$ where

$$Q = \mathbb{E} \left[\sum_{t=1}^T \tilde{p}_t(1 | S_t) (1 - \tilde{p}_t(1 | S_t)) f_t(S_t) f_t(S_t)^\top \right]$$

and

$$W = \mathbb{E} \left[\sum_{t=1}^T W_{t,j} \times W_{t,\Delta,j} \epsilon_{t,j} (A_{t,j} - \tilde{p}_t(1 | S_t)) f_t(S_t) \right. \\ \left. \times \sum_{t=1}^T W_{t,\bar{j}} \times W_{t,\Delta,\bar{j}} \epsilon_{t,\bar{j}} (A_{t,\bar{j}} - \tilde{p}_t(1 | S_t)) f_t(S_t)^\top \right],$$

where $\epsilon_{t,j} = Y_{t,\Delta,j} - g_t(H_t)^\top \alpha^* - (A_{t,j} - \tilde{p}_t(1 | S_t)) f_t(S_t)^\top \beta^*$, α^* minimizes the least-squares criterion $\mathbb{E} \left[G_m^{-1} \sum_{j=1}^{G_m} \sum_{t=1}^T W_{t,j} W_{t,\Delta,j} (Y_{t,\Delta,j} - g_t(H_t)^\top \alpha)^\top \right]$, and both J and \bar{J} are independent randomly sampled indices from the same cluster.

In practice, plug-in estimates \hat{Q} and \hat{W} are used to estimate the covariance structure; Appendix F presents their estimates with small-sample adjustments.

Remark 4.3.—(*L₂ Projection Interpretation*) Importantly, Assumption 4.1 is not required. That is, we can follow [18, 19, 20, 5] and others in using $f_t(s)^\top \beta$ as a working model for $\beta_{p,\pi,\Delta}(t; s)$. Specifically, $\hat{\beta}$ is a solution to the weighted least-squares projection

$$\beta^* = \operatorname{argmin}_{\beta} \mathbb{E} \left[\frac{1}{G} \sum_{j=1}^G \sum_{t=1}^T \tilde{p}_t(1 | S_t) (1 - \tilde{p}_t(1 | S_t)) (\beta(t; S_t) - f_t(S_t)^\top \beta)^2 \right].$$

Here, the weight is the variance of the numerator in the weight $W_{t,j}$. To interpret as a projection or as a correctly specified causal effect can be viewed as a bias-variance trade-off. The projection interpretation guarantees well-defined parameter interpretation in practice where Assumption 4.1 is unlikely to hold. See [Sec. 3.1, pp.9–10 20] for a discussion of the use of projections in causal versus predictive settings.

Appendix I presents semiparametric efficiency theory in the special case of $S_t = H_t$.

4.2. Connection to the Standard MRT Analysis.

A natural question is whether there are conditions such that the standard MRT analysis presented in Section 2.2 is equivalent to the proposed direct effect analysis. Lemma 4.4 proves that, under certain conditions, an equivalence of estimates and asymptotic variances is guaranteed.

Lemma 4.4.—Consider the direct effect when the moderator is defined on the individual (i.e., $S_{t,j}$), and the randomization probabilities only depend on the individual's observed history, i.e., $p(A_{t,j} | H_t) = p(A_{t,j} | H_{t,j})$. If cluster size is constant (i.e., $G_m \equiv G$), then the point estimates from (3) and (5) are equal for any sample size. Moreover, if

$$\mathbb{E}[\mathbb{E}[W_{t,\Delta,j} \epsilon_{t,j} \times W_{t',\Delta,j} \epsilon_{t',j'} | H_{t,j}, A_{t,j} = a, H_{t',j'}, A_{t',j'} = a'] | S_{t,j}, S_{t',j'}] \quad (8)$$

equals $\psi(S_{t,j}, S_{t',j'})$ for some function ψ , i.e., the cross-terms are constant in a and a' , where $\epsilon_{t,j}$ is the error defined in Lemma 4.2, then the estimators share the same asymptotic variance.

Proof of Lemma 4.4 can be found in Appendix E. Here, a class of random effect models is introduced to help with interpretation of the sufficient condition (8). Specifically, for participant j at decision time t , let $\Delta = 1$ and suppose the generative model for the proximal response is

$$Y_{t,1,j} = g_t(H_{t,j})^\top \alpha + \underbrace{Z_{t,j}^\top b_g}_{(I)} + (A_{t,j} - p_t(1 | H_{t,j}))(f_t(H_{t,j})^\top \beta + \underbrace{Z_{t,j}^\top \tilde{b}_g}_{(II)}) + e_{t,j}$$

where (I) and (II) are random effects with design matrix $Z_{t,j}$, $\mathbb{E}[f_t(H_{t,j})^\top \beta | S_{t,j}] = f_t(S_{t,j})^\top \beta$, and $e_{t,j}$ is a participant-specific error term. The treatment effect conditional on the complete observed history and the random effects is $f_t(H_{t,j})^\top \beta + Z_{t,j}^\top \tilde{b}_g$, which implies the marginal causal effect is $f_t(S_{t,j})^\top \beta$ so Assumption 4.1 holds. Random effects in (I) allow for cluster-level variation in baseline values of the proximal response, while random effects in (II) allow for cluster-level variation in the fully-conditional treatment effect. Given the above generative model, sufficient condition (8) holds if $\tilde{b}_g \equiv 0$, i.e., when the treatment effect does not exhibit cluster-level variation. For this reason, (8) is referred to as a treatment effect heterogeneity condition. The condition motivates our simulation study in Section 5, which empirically supports this conclusion of equivalence.

4.3. Pairwise Indirect Causal Excursion Effect Estimation.

Assumption 4.5.—Assume the pairwise indirect causal excursion effect

$\beta_{p,\pi,\Delta}^{(IE)}(t; s) = f_t(s)^\top \beta^{* *}$, where $f_t(s) \in \mathbb{R}^q$ is a q -dimensional vector function of s and time t .

Consider inference on the q -dimensional parameter $\beta^{* *}$. Define the weight $W_{t,j,j'}$ at decision time t for the j th individual as equal to $\frac{\tilde{p}_t(A_{t,j}, A_{t,j'} | S_t)}{p_t(A_{t,j}, A_{t,j'} | H_t)}$ where $\tilde{p}_t(a, a' | S_t) \in (0, 1)$ is arbitrary as long as it does not depend on terms in H_t other than S_t , and $p_t(A_{t,j}, A_{t,j'} | H_t)$ is the marginal probability that individuals j and j' receive treatments $A_{t,j}$ and $A_{t,j'}$ respectively given H_t . Here we consider an estimator which is the minimizer of the following cluster-based weighted-centered least-squares (C-WCLS) criterion:

$$\mathbb{P}_M \left[\frac{1}{G_m(G_m - 1)} \sum_{j \neq j'} \sum_{t=1}^T W_{t,j,j'} \times W_{t,\Delta,j,j'} \times (Y_{t,\Delta,j} - g_t(H_t)^\top \alpha - (1 - A_{t,j})(A_{t,j'} - \tilde{p}_t^*(1 | S_t))f_t(S_t)^\top \beta)^2 \right] \quad (9)$$

where $\tilde{p}_t^*(1 | S_t) = \frac{\tilde{p}_t(0, 1 | S_t)}{\tilde{p}_t(0, 0 | S_t) + \tilde{p}_t(0, 1 | S_t)}$ and

$W_{t,\Delta,j,j'} = \prod_{u=t+\Delta-1}^t \pi(A_{u,j}, A_{u,j'} | H_u) / p(A_{u,j}, A_{u,j'} | H_u)$. If an individual's randomization probabilities only depends on their own observed history then $\tilde{p}_t^*(1 | S_{t,j}) = \tilde{p}_t(1 | S_{t,j})$ and the weight $W_{t,\Delta,j,j'} = W_{t,\Delta,j} \times W_{t,\Delta,j'}$. In Appendix A, we prove the following result.

Lemma 4.6.—Under Assumption 4.5, then, under invertibility and moment conditions, the estimator $\hat{\beta}^{(IE)}$ that minimizes (9) satisfies $\sqrt{M}(\hat{\beta}^{(IE)} - \beta^{\star \star}) \rightarrow N(0, Q^{-1}WQ^{-1})$ where

$$Q = \mathbb{E} \left[\sum_{t=1}^T (\tilde{p}_t(0, 0 | S_t) + \tilde{p}_t(0, 1 | S_t)) \tilde{p}_t^*(1 | S_t) (1 - \tilde{p}_t^*(1 | S_t)) f_t(S_t) f_t(S_t)^\top \right]$$

and

$$W = \mathbb{E} \left[\sum_{t=1}^T W_{i,j,j'} W_{i,\Delta,j,j'} \epsilon_{i,j,j'} (1 - A_{i,j}) (A_{i,j} - \tilde{p}_t^*(1 | S_t)) f_t(S_t) \right. \\ \left. \times \sum_{t=1}^T W_{i,\tilde{j},\tilde{j}'} \times W_{i,\Delta,\tilde{j},\tilde{j}'} \epsilon_{i,\tilde{j},\tilde{j}'} (1 - A_{i,\tilde{j}}) (A_{i,\tilde{j}} - \tilde{p}_t^*(1 | S_t)) f_t(S_t)^\top \right]$$

where $\epsilon_{i,j,j'} = Y_{i,\Delta,j} - g_i(H_i)^\top \alpha^{\star \star} - (1 - A_{i,j})(A_{i,j} - \tilde{p}_t^*(1 | S_t)) f_t(S_t)^\top \beta^{\star \star}$, $\alpha^{\star \star}$ minimizes the least-squares criterion $\mathbb{E} \left[\frac{1}{G_m(G_m - 1)} \sum_{j \neq j'} \sum_{t=1}^T W_{i,j,j'} W_{i,\Delta,j,j'} (Y_{i,\Delta,j} - g_i(H_i)^\top \alpha)^2 \right]$, and both (J, J') and (\tilde{J}, \tilde{J}') are independently, randomly sampled pairs from the cluster.

Remark 4.7.—In Appendix H, variances are re-derived in the general setting where the numerators $\tilde{p}_t(a | S_t)$ and $\tilde{p}_t(a, a' | S_t)$ are estimated using the observed MRT data.

5. SIMULATIONS

To evaluate the proposed estimator, we extend the simulation setup in [3]. We first present a base data generation model, which is to be extended in four scenarios. In this section, we focus on presenting simulation settings and results for lag-1 proximal responses ($\Delta = 1$); see Appendix D for scenarios under $\Delta > 1$ with similar conclusions about the relative advantage of the proposed method. Consider an MRT with known randomization probability and the observation vector O_t being a single state variable $S_t \in \{-1, 1\}$ at each decision time t . Let

$$Y_{t,1} = \theta_1 \{S_t - \mathbb{E}[S_t | A_{t-1}, H_{t-1}]\} + \{A_t - p_t(1 | H_t)\} (\beta_{10} + \beta_{11} S_t) + e_{t+1}. \quad (10)$$

The randomization probability is $p_t(1 | H_t) = \text{expit}(\eta_1 A_{t-1} + \eta_2 S_t)$ where $\text{expit}(x) = 1 + \exp(-x)^{-1}$; the state dynamics are given by $\mathbb{P}(S_t = 1 | A_{t-1}, H_{t-1}) = \text{expit}(\xi A_{t-1})$ with $A_0 = 0$, and the independent error term satisfies $e_t \sim \mathcal{N}(0, 1)$ with $\text{Corr}(e_u, e_t) = 0.5^{|u-t|/2}$. As in [3], we set $\theta_1 = 0.8$, $\xi = 0$, $\eta_1 = -0.8$, $\eta_2 = 0.8$, $\beta_{10} = -0.2$, and $\beta_{11} = 0.2$. Because $\xi = 0$, the marginal proximal effect is equal to $\beta_{10} + \beta_{11} \mathbb{E}[S_t] = \beta_{10} = -0.2$. In extending the data generation model to clustered settings, we conducted simulation studies with 25, 50, 100 clusters with equal sizes (15 or 25); here, we report results with 50 clusters showing the relative advantage of C-WCLS over WCLS. A more complete set of simulation results with similar findings can be found in Appendix C.

Simulation Scenario I.

The first scenario estimates the marginal proximal effect when an individual-level moderator exists and proximal responses share a random cluster-level intercept term that does not interact with treatment. The data generative model (10) incorporates a cluster-level random-intercept $e_g \sim \mathcal{N}(0, 0.5)$. Table 1 presents the results, which shows both WCLS and the proposed C-WCLS approach are nearly unbiased and have proper coverage rates. This is in line with Lemma 4.4 stating asymptotic equivalence under no cluster-level treatment heterogeneity.

Simulation Scenario II.

In the second scenario, we extend Scenario I to include a random cluster-level intercept term that interacts with treatment by considering the linear model with the additional term $b_g \times (A_{t,j} - p_t(1 | H_{t,j}))$ where $b_g \sim \mathcal{N}(0, 0.1)$. Table 1 presents the results which demonstrate that if cluster-level random effects interact with treatment, then both methods produce nearly unbiased estimates of the marginal proximal effect but only the proposed method achieves the nominal 95% coverage probability. To further demonstrate this, Figure 2 presents nominal coverage as a function of the ratio of the variance of b_g over the variance of e_g as well as group size respectively.

Simulation Scenario III.

In the third scenario, the treatment effect for an individual is assumed to depend on the average state of all individuals in the cluster, i.e., define the cluster-level moderator $\bar{S}_{t,g} = \frac{1}{G_g} \sum_{j=1}^{G_g} S_{t,j}$ and consider the linear model from Scenario II with the additional term $\bar{S}_{t,g} \times (A_{t,j} - p_t(1 | H_{t,j}))$. The proposed estimator again achieves the nominal 95% coverage probability while the WCLS method does not (see Scenario III, Table 1).

Simulation Scenario IV.

The fourth scenario considers the indirect effect. For individual j at decision point t , define the total effect to be $TE_{t,j} = \sum_{j' \neq j} \{A_{t,j'} - \tilde{p}_{t,j'}(1 | H_{t,j'})\}(\beta_{20} + \beta_{21}S_{t,j'})$, where $\beta_{20} = -0.1$ and $\beta_{21} = 0.2$. The generative model is then given by:

$$Y_{t,1,j} = (-0.2 + b_g + 0.2 \cdot \bar{S}_{t,g}) \times \{A_{t,j} - p_t(1 | H_{t,j})\} + 0.8S_{t,j} + TE_{t,j} + e_g + e_{t+1,j}.$$

This model implies a marginal pairwise indirect effect equal to $\beta^{(IE)} = \beta_{20} = -0.1$. Table 1 presents simulation results which shows that the proposed indirect estimator exhibited nearly no bias and achieved the nominal coverage probability.

6. CASE STUDY: INTERN HEALTH STUDY

The Intern Health Study (IHS) was a 6-month MRT on 1,562 medical interns where four types of weekly notification - mood, activity, sleep, or none – were randomly assigned with equal probability to each subject [10]; see Section 2.3 for prior discussion. In IHS, 285 institutions and 24 specialties were observed. Here, we assess the effect of the three types of

notifications (mood, activity, and sleep) compared to no notifications on the weekly average of self-reported mood scores, log step-count and log sleep minutes for the population of interns. Due to high levels of missing data, weekly proximal responses were multiply imputed. See [10] for further details.

Let $t = 1, \dots, T$ denote the weekly decision points at which the individual is randomized to the various types of notifications. The three proximal responses are the average weekly mood score, which is reported on a Likert scale taking values from 1 to 10 (higher scores mean better mood), log step count and log sleep minutes respectively. Notifications are collapsed to a binary variable, i.e., $A_{t,j} = 1$ if the individual was assigned to receive any notifications on week t ; otherwise, $A_{t,j} = 0$. We start by defining clusters based on medical specialty as we saw effect heterogeneity by specialty in Figure 1. The average cluster size was 65; the first and third quartile were 7 and 113 respectively, with maximum and minimum sizes of 333 and 1. For every individual in each cluster at each decision point, we compute the average prior weekly proximal response for all others in the cluster, denoted $\bar{Y}_{t,-j}$ for the j th individual in the cluster. We conducted analyses under lag $\Delta = 1$ and $\Delta = 2$. Here we report results under $\Delta = 1$; see Appendix G for results under $\Delta = 2$ for two choices of reference policy π . Under $\Delta = 1$, we consider two moderation analyses that can both be expressed as $\beta(t; S_t) = \beta_0 + \beta_1 \cdot Y_{t,j} + \beta_2 \bar{Y}_{t,-j}$.

The first set of moderation analyses considers the standard moderation analysis where only individual-level moderators are included (i.e., $\beta_2 = 0$). Figure 3 visualizes the estimates across the range of prior week's proximal response for both our proposed approach and the WCLS approach from [3], and the numerical output can be found in Appendix G.1. In comparison, C-WCLS produces larger variance estimates for all proximal responses as expected. The effects do not change too much for the average weekly mood and sleep analysis; however, the significant effect of messages on weekly log step count under the traditional MRT analysis becomes insignificant when accounting for cluster effects.

The second moderation analysis lets β_2 be a free parameter, enabling novel moderation analyses that accounts for the average weekly previous proximal responses of other individuals. Table 2 presents the results. Here, we see that the new term β_2 is negative but insignificant. The results suggest the average proximal responses of others in the cluster have a limited moderation effect. To conclude, the impact of a notification on mood is larger while the individual's score from previous week is low. Similar results hold for the log step-count analysis.

Finally, we consider indirect moderation effect analyses. In this analysis, clusters are defined based on medical specialty and institution because interference was only likely when interns are in close geographic proximity. Here, we consider the marginal indirect effect (e.g., no moderators) both when the individual did not receive the intervention and when the individual did receive an intervention at decision time t . Table 2 presents the results. In this case, the estimated indirect effects are much weaker than the direct effects. Even a weak effect may be unexpected as none of the content in the push notifications was aimed at impacting other individuals' behavior. For all the proximal responses, we see limited

evidence of an indirect effect. This implies that the scientific team, when building an optimal intervention package, may ignore these indirect effects and focus solely on the individual who receives these types of push notifications.

7. DISCUSSION

We revisited causal excursion effects in the presence of *a priori* known clusters in sequential treatment settings where outcome of interest is measured at all decision points. In particular, we formalized both direct and indirect excursion effects in the context of MRT to account for potential interference. We studied their identifications and proposed consistent and robust inference methods. In practice, the effects described in this paper are most important when using MRT data to build optimized just-in-time adaptive interventions (JITAs) for deployment in an mHealth package. Specifically, the estimation procedure for the direct excursion effect accounts for within-cluster correlation in the proximal responses which helps the scientific team avoid making erroneous conclusions about intervention effectiveness using standard MRT methods. Moreover, estimation of indirect effects allows the scientific team to answer questions about impact of interventions on other members of the same cluster. Use of these methods provides empirical evidence for the scientific team to include or exclude intervention components that may have had unanticipated second order effects, or potentially lead to novel ways to improve the intervention component by revising the intervention to more explicitly account for cluster-level interference. While this work represents a major step forward in the analysis of micro-randomized trial data, further work is required. Specifically, useful extensions include accounting for overlapping communities and/or network (rather than cluster-only) structure [21, 22], accounting for general non-continuous proximal responses such as binary or count outcomes [4], penalization of the working model to allow for high-dimensional moderators, and a method to use the proposed approach to form warm-start policies at the individual level while accounting for group level information [23].

Appendix A.: TECHNICAL DETAILS

Lemma 3.3. We establish Lemma 3.3 for the direct effect (5). For $a_s \in \{0, 1\}^G$, we consider

$$\begin{aligned} & \mathbb{E} \left[\left(\prod_{s=1}^{t-1} p_s(a_s | H_s(\bar{a}_{s-1})) \right) \left(\prod_{j' \neq j} \prod_{s=t}^{t+\Delta-1} p_s(a_{s,j'} | H_s(\bar{a}_{s-1})) \right) \right. \\ & \quad \left. \left(\prod_{s=t}^{t+\Delta-1} \pi_s(a_{s,j} | H_s(\bar{a}_{s-1})) \right) Y_{t,\Delta,j}(\bar{a}_{t+\Delta-1,-j}, (\bar{a}_{t-1,j}, a, a_{t+1:(t+\Delta-1),j})) \mathbf{1}_{S_t(\bar{a}_t)=s} \right) \right] \\ &= \mathbb{E} \left[\left(\prod_{s=1}^{t-1} p_s(a_s | H_s(\bar{a}_{s-1})) \right) \mathbf{1}_{S_t(\bar{a}_t)=s} \left(\prod_{j' \neq j} \prod_{s=t}^{t+\Delta-1} p_s(a_{s,j'} | H_s(\bar{a}_{s-1})) \right) \right. \\ & \quad \left. \mathbb{E} \left[\left(\prod_{s=t}^{t+\Delta-1} \pi_s(a_{s,j} | H_s(\bar{a}_{s-1})) \right) Y_{t,\Delta,j}(\bar{a}_{t+\Delta-1,-j}, (\bar{a}_{t-1,j}, a, a_{t+1:(t+\Delta-1),j})) \mid H_t(\bar{a}_{t-1}) \right] \right] \end{aligned}$$

$$= \mathbb{E} \left[\left(\prod_{s=1}^{t-1} p_s(a_s | H_s(\bar{a}_{s-1})) \right) \mathbf{1}_{S_t(\bar{a}_t)=s} \left(\prod_{j' \neq j}^{t+\Delta-1} \prod_{s=t}^{t+\Delta-1} p_s(a_{s,j'} | H_s(\bar{a}_{s-1})) \right) \right. \\ \left. \mathbb{E} \left[\left(W_{t,\Delta,j}(\bar{a}_{t+\Delta-1}) \prod_{s=t}^{t+\Delta-1} p_s(a_s | H_s(\bar{a}_{s-1})) \right) Y_{t,\Delta,j}(\bar{a}_{t+\Delta-1}, -j, (\bar{a}_{t-1,j}, a, a_{t+1:(t+\Delta-1),j})) \mid H_t(\bar{a}_{t-1}) \right] \right]$$

since the history H_t includes the moderator variable S_t at time t . By consistency, $H_t(\bar{A}_{t-1}) = H_t$. Moreover, sequential ignorability implies that

$$\mathbb{E} \left[\left(W_{t,\Delta,j}(\bar{a}_{t+\Delta-1}) \prod_{s=t}^{t+\Delta-1} p_s(a_s | H_s(\bar{a}_{s-1})) \right) Y_{t,\Delta,j}(\bar{a}_{t+\Delta-1}, -j, (\bar{a}_{t-1,j}, a, a_{t+1:(t+\Delta-1),j})) \mid H_t \right] \\ = \mathbb{E} \left[\left(W_{t,\Delta,j}(\bar{a}_{t+\Delta-1}) \prod_{s=t}^{t+\Delta-1} p_s(a_s | H_s(\bar{a}_{s-1})) \right) Y_{t,\Delta,j}(\bar{a}_{t+\Delta-1}, -j, (\bar{a}_{t-1,j}, a, a_{t+1:(t+\Delta-1),j})) \mid H_t, A_{t,j} = a \right]$$

It also implies that $\mathbb{E}[1[A_{t+k,j} = a] \mid H_{t+k}] \cdot \mathbb{E}[Y_{t,\Delta,j} \mid H_{t+k}] = \mathbb{E}[Y_{t,\Delta,j} 1[A_{t+k,j} = a] \mid H_{t+k}]$. Summing over all potential outcomes yields

$$\mathbb{E} \left[\sum_{\bar{a}_{t-1}, \bar{a}_{t+1:(t+\Delta-1)}} \left(\prod_{s=1}^{t-1} p_s(a_s | H_s) \right) \left(\prod_{j' \neq j} p_s(a_{t,j'} | H_t) \right) \mathbf{1}_{S_t(\bar{a}_t)=s} \right. \\ \left. \times \mathbb{E} \left[\left(\prod_{s=t}^{t+\Delta-1} \pi_s(a_{s,j} | H_t) \right) Y_{t,\Delta,j}(\bar{a}_{t+\Delta-1}, -j, (\bar{a}_{t-1,j}, a, a_{t+1:(t+\Delta-1),j})) \mid H_t, A_{t,j} = a \right] \right] \\ = \mathbb{E} \left[\sum_{\bar{a}_{t-1}, \bar{a}_{t+1:(t+\Delta-1)}} \left(\prod_{s=1}^{t-1} p_s(a_s | H_s) \right) \left(\prod_{j' \neq j} p_s(a_{t,j'} | H_t) \right) \mathbf{1}_{S_t=s} \right. \\ \left. \times \mathbb{E} \left[\left(\prod_{s=t}^{t+\Delta-1} p_s(a_s | H_t) \right) \times W_{t,\Delta,j}(\bar{a}_{t+\Delta-1}) \right. \right. \\ \left. \left. \times Y_{t,\Delta,j}(\bar{a}_{t+\Delta-1}, -j, (\bar{a}_{t-1,j}, a, a_{t+1:(t+\Delta-1),j})) \mid H_t, A_{t,j} = a \mid S_t = s \right] \right] \\ \Rightarrow \mathbb{E}_{p,\pi} [Y_{t,\Delta,j}(\bar{A}_{t+\Delta-1}, -j, (\bar{A}_{t-1,j}, a, \tilde{A}_{t+1:(t+\Delta-1)}) \mid S_t(\bar{A}_{t-1}) = s] = \mathbb{E}[\mathbb{E}[W_{t,\Delta,j} Y_{t,\Delta,j} \mid H_t, A_{t,j} = a] \mid S_t = s].$$

Averaging over individuals in the group $j \in [G]$ group size completes the proof. The proof for the indirect effect follows the exact same structure. \square

Appendix B.: LEMMA 4.2

We next provide a detailed proof of asymptotic normality and consistency for the weighted-centered least squares estimator.

Consistency for direct and indirect effects.

The solutions $(\hat{\alpha}, \hat{\beta})$ that minimize equation (7) are consistent estimators for the solutions that minimize the following

$$\mathbb{E} \left[\frac{1}{G} \sum_{j=1}^G \sum_{t=1}^T W_{t,j} \times W_{t,\Delta,j} \left(Y_{t,\Delta,j} - g_t(H_t)^\top \alpha - (A_{t,j} - \tilde{p}_t(1 | S_t)) f_t(S_t)^\top \beta \right)^2 \right]$$

Differentiating the above equation with respect to α yields a set of p estimating equations.

$$0_q = \mathbb{E} \left[\frac{1}{G} \sum_{j=1}^G \sum_{t=1}^T W_{t,j} \times W_{t,\Delta,j} \left(Y_{t,\Delta,j} - g_t(H_t)^\top \alpha - (A_{t,j} - \tilde{p}_t(1 | S_t)) f_t(S_t)^\top \beta \right) g_t(H_t) \right]$$

We note that

$$\mathbb{E} \left[W_{t,j} W_{t,\Delta,j} (A_{t,j} - \tilde{p}_t(1 | S_t)) f_t(S_t)^\top \beta \mid H_t \right] = 0.$$

Therefore, we have,

$$0_p = \mathbb{E} \left[\frac{1}{G} \sum_{j=1}^G \sum_{t=1}^T \left(g_t(H_t) \mathbb{E} [W_{t,j} W_{t,\Delta,j} Y_{t,\Delta,j} \mid H_t] - g_t(H_t) g_t(H_t)^\top \alpha \right) \right]$$

$$\Rightarrow \alpha = \mathbb{E} \left[\frac{1}{G} \sum_{j=1}^G \sum_{t=1}^T g_t(H_t) g_t(H_t)^\top \right]^{-1} \mathbb{E} \left[\frac{1}{G} \sum_{j=1}^G \sum_{t=1}^T g_t(H_t) \mathbb{E} [W_{t,j} W_{t,\Delta,j} Y_{t,\Delta,j} \mid H_t] \right]$$

We note that

$$\mathbb{E} \left[W_{t,j} W_{t,\Delta,j} (A_{t,j} - \tilde{p}_t(1 | S_t)) g_t(H_t)^\top \alpha \right] = 0, \quad \text{and}$$

$$\mathbb{E} [W_{t,j} W_{t,\Delta,j} (A_{t,j} - \tilde{p}_t(1 | S_t)) Y_{t,\Delta,j}] = \tilde{p}_t(1 | S_t) (1 - \tilde{p}_t(1 | S_t)) \beta_{p,\pi,\Delta}(t; S_t), \quad \text{and}$$

$$\mathbb{E} \left[W_{t,j} W_{t,\Delta,j} (A_{t,j} - \tilde{p}_t(1 | S_t))^2 \mid S_t \right] = \tilde{p}_t(1 | S_t) (1 - \tilde{p}_t(1 | S_t))$$

Now differentiating with respect to β yields

$$0_q = \mathbb{E} \left[\sum_{t=1}^T W_{t,j} \left(Y_{t,\Delta,j} - g_t(H_t)^\top \alpha - (A_{t,j} - \tilde{p}_t(1 | S_t)) f_t(S_t)^\top \beta \right) (A_{t,j} - \tilde{p}_t(1 | S_t)) f_t(S_t) \right]$$

$$0_q = \mathbb{E} \left[\sum_{t=1}^T \tilde{p}_t(1 | S_t)(1 - \tilde{p}_t(1 | S_t)) (\beta_{p,\pi,\Delta}(t; S_t) - f_t(S_t)^\top \beta^*) f_t(S_t) \right]$$

Then we have

$$\beta^* = \mathbb{E} \left[\sum_{t=1}^T \tilde{p}_t(1 | S_t)(1 - \tilde{p}_t(1 | S_t)) f_t(S_t) f_t(S_t)^\top \right]^{-1} \mathbb{E} \left[\sum_{t=1}^T \tilde{p}_t(1 | S_t)(1 - \tilde{p}_t(1 | S_t)) f_t(S_t) \beta_{p,\pi,\Delta}(t; S_t) \right]$$

Under assumption 4.1, we have that $\beta = \beta^*$ which guarantees consistency.

We next consider the indirect effect estimator. Recall that

$$\tilde{p}_t^*(1 | S_t) = \frac{\tilde{p}_t(0, 1 | S_t)}{\tilde{p}_t(0, 0 | S_t) + \tilde{p}_t(0, 1 | S_t)}$$

is the replacement for $\tilde{p}_t(1 | S_t)$ in the direct effect for centering. If we make the assumption that $\tilde{p}_t(0, 1 | S_t) = \tilde{p}_t(0 | S_t) \tilde{p}_t(1 | S_t)$ then $\tilde{p}_t^*(1 | S_t) = \tilde{p}_t(1 | S_t)$; however, we provide the proof in complete generality. The estimates that minimize equation (9) are consistent estimators for the solutions that minimize the following

$$\mathbb{E} \left[\sum_{t=1}^T W_{t,J,J} W_{t,\Delta,J,J} (Y_{t,\Delta,J} - g_t(H_t)^\top \alpha - (1 - A_{t,J})(A_{t,J} - \tilde{p}_t^*(1 | S_t)) f_t(S_t)^\top \beta)^2 \right]$$

Differentiating the above equation with respect to α yields a set of p estimating equations.

$$0_p = \mathbb{E} \left[\sum_{t=1}^T W_{t,J,J} W_{t,\Delta,J,J} (Y_{t,\Delta,J} - g_t(H_t)^\top \alpha - (1 - A_{t,J})(A_{t,J} - \tilde{p}_t^*(1 | S_t)) f_t(S_t)^\top \beta) g_t(H_t) \right]$$

We note that

$$\mathbb{E} [W_{t,J,J} W_{t,\Delta,J,J} (1 - A_{t,J})(A_{t,J} - \tilde{p}_t^*(1 | S_t)) f_t(S_t)^\top \beta | H_t] = 0.$$

Therefore, we have,

$$\begin{aligned} 0_p &= \mathbb{E} \left[\sum_{t=1}^T (g_t(H_t) \mathbb{E}[W_{t,J,J} W_{t,\Delta,J,J} Y_{t,\Delta,J} | H_t] - g_t(H_t) g_t(H_t)^\top \alpha) \right] \\ \Rightarrow \alpha &= \mathbb{E} \left[\frac{1}{G} \sum_{j=1}^G \sum_{t=1}^T g_t(H_t) g_t(H_t)^\top \right]^{-1} \mathbb{E} \left[\sum_{t=1}^T g_t(H_t) \mathbb{E}[W_{t,J,J}, W_{t,\Delta,J,J} Y_{t,\Delta,J} | H_t] \right] \end{aligned}$$

First, we show that

$$\begin{aligned}
 & \mathbb{E}[W_{i,j,j}W_{i,\Delta,j,j}(1-A_{i,j})(A_{i,j}-\tilde{p}_i^*(1|S_i)) | H_i] \\
 &= \mathbb{E}[W_{i,j,j}(1-A_{i,j})(A_{i,j}-\tilde{p}_i^*(1|S_i)) | H_i] \\
 &= \sum_{a' \in \{0,1\}} \mathbb{E}[\tilde{p}_i(0,a' | S_i)(a' - \tilde{p}_i^*(1|S_i)) | H_i, A_i = 0, A_{i,j} = a'] \\
 &= \tilde{p}_i(0,1 | S_i) \left(1 - \frac{\tilde{p}_i(0,1 | S_i)}{\tilde{p}_i(0,0 | S_i) + \tilde{p}_i(0,1 | S_i)}\right) - \tilde{p}_i(0,0 | S_i) \frac{\tilde{p}_i(0,1 | S_i)}{\tilde{p}_i(0,0 | S_i) + \tilde{p}_i(0,1 | S_i)} = 0
 \end{aligned}$$

and

$$\begin{aligned}
 & \mathbb{E}[W_{i,j,j}W_{i,\Delta,j,j}(1-A_{i,j})(A_{i,j}-\tilde{p}_i^*(1|S_i))^2 | H_i] \\
 &= \mathbb{E}[W_{i,j,j}(1-A_{i,j})(A_{i,j}-\tilde{p}_i^*(1|S_i))^2 | H_i] \\
 &= \tilde{p}_i(0,1 | S_i) \left(\frac{\tilde{p}_i(0,0 | S_i)}{\tilde{p}_i(0,0 | S_i) + \tilde{p}_i(0,1 | S_i)}\right)^2 + \tilde{p}_i(0,0 | S_i) \left(\frac{\tilde{p}_i(0,1 | S_i)}{\tilde{p}_i(0,0 | S_i) + \tilde{p}_i(0,1 | S_i)}\right)^2 \\
 &= (\tilde{p}_i(0,0 | S_i) + \tilde{p}_i(0,1 | S_i))\tilde{p}_i^*(1|S_i)(1 - \tilde{p}_i^*(1|S_i)).
 \end{aligned}$$

This implies that

$$\mathbb{E}[W_{i,j,j}W_{i,\Delta,j,j}(1-A_{i,j})(A_{i,j}-\tilde{p}_i^*(1|S_i))g_i(H_i)^\top \alpha] = 0, \quad \text{and}$$

$$\frac{\mathbb{E}[W_{i,j,j}W_{i,\Delta,j,j}(1-A_{i,j})(A_{i,j}-\tilde{p}_i^*(1|S_i))Y_{i,\Delta,j}]}{\tilde{p}_i(0,0 | S_i) + \tilde{p}_i(0,1 | S_i)} = \tilde{p}_i^*(1|S_i)(1 - \tilde{p}_i^*(1|S_i))\beta_{p,\pi,\Delta}^{(E)}(t; S_i).$$

Now differentiating with respect to β yields

$$0_q = \mathbb{E} \left[\sum_{t=1}^T (\tilde{p}_i(0,0 | S_i) + \tilde{p}_i(0,1 | S_i))\tilde{p}_i^*(1|S_i)(1 - \tilde{p}_i^*(1|S_i)) \left(\beta_{p,\pi,\Delta}^{(E)}(t; S_i) - f_i(S_i)^\top \beta^* \right) f_i(S_i) \right]$$

Under assumption 4.5, we have that $\beta = \beta^*$ which guarantees consistency. \square

Asymptotic Normality.

We now consider the issue of asymptotic normality. First, let

$$\epsilon_{i,\Delta,j} = Y_{i,\Delta,j} - g_i(H_i)^\top \alpha^* - (A_{i,j} - \tilde{p}_i(1 | S_i)) f_i(S_i)^\top \beta^*,$$

$\hat{\theta} = (\hat{\alpha}, \hat{\beta})$, and $\theta^* = (\alpha^*, \beta^*)$. Since $S_i \subset H_i$ define $h_{i,j}(H_i)^\top = (g_i(H_i)^\top, (A_{i,j} - \tilde{p}_i(1 | S_i)) f_i(S_i)^\top)$.

Then

$$\begin{aligned} \sqrt{M}(\hat{\theta} - \theta^*) &= \sqrt{M} \left\{ \mathbb{P}_M \left(\frac{1}{G_m} \sum_{j=1}^{G_m} \sum_{t=1}^T W_{t,j} W_{t,\Delta,j} h_{i,j}(H_t) h_{i,j}(H_t)^\top \right)^{-1} \right. \\ &\quad \left. \left[\mathbb{P}_M \left(\frac{1}{G_m} \sum_{j=1}^{G_m} \sum_{t=1}^T W_{t,j} W_{t,\Delta,j} Y_{t,\Delta,j} h_{i,j}(H_t) \right) \right. \right. \\ &\quad \left. \left. - \mathbb{P}_M \left(\frac{1}{G_m} \sum_{j=1}^{G_m} \sum_{t=1}^T W_{t,j} W_{t,\Delta,j} h_{i,j}(H_t) h_{i,j}(H_t)^\top \right) \theta^* \right] \right\} \\ &= \sqrt{M} \left\{ E \left[\frac{1}{G} \sum_{j=1}^G \sum_{t=1}^T W_{t,j} W_{t,\Delta,j} h_{i,j}(H_t) h_{i,j}(H_t)^\top \right]^{-1} \right. \\ &\quad \left. \left[\mathbb{P}_M \left(\frac{1}{G_m} \sum_{j=1}^{G_m} \sum_{t=1}^T W_{t,j} W_{t,\Delta,j} \epsilon_{t,\Delta,j} h_{i,j}(H_t) \right) \right] \right\} + o_p(\mathbf{1}) \end{aligned}$$

By definitions of α^* and β^* and the previous consistency argument

$$E \left[\frac{1}{G} \sum_{j=1}^G \sum_{t=1}^T W_{t,j} W_{t,\Delta,j} h_{i,j}(H_t) h_{i,j}(H_t)^\top \right] = 0$$

Then under moments conditions, we have asymptotic normality with variance Σ_θ given by

$$\begin{aligned} \Sigma_\theta &= E \left[\frac{1}{G} \sum_{j=1}^G \sum_{t=1}^T W_{t,j} W_{t,\Delta,j} h_{i,j}(H_t) h_{i,j}(H_t)^\top \right]^{-1} \\ &\quad E \left[\frac{1}{G} \sum_{j=1}^G \sum_{t=1}^T W_{t,j} W_{t,\Delta,j} \epsilon_{t,\Delta,j} h_{i,j}(H_t) \times \frac{1}{G} \sum_{j=1}^G \sum_{t=1}^T W_{t,j} W_{t,\Delta,j} \epsilon_{t,\Delta,j} h_{i,j}(H_t)^\top \right] \\ &\quad E \left[\frac{1}{G} \sum_{j=1}^G \sum_{t=1}^T W_{t,j} W_{t,\Delta,j} h_{i,j}(H_t) h_{i,j}(H_t)^\top \right]^{-1} \end{aligned}$$

Due to centering, the expectation of the matrix $W_{t,j} h_{i,j}(H_t) h_{i,j}(H_t)^\top$ is block diagonal and the sub-covariance matrix Σ_β can be extracted and is equal to

$$\Sigma_\theta = \left[\sum_{t=1}^T E \left[(A_{t,j} - \tilde{p}_t(1 | S_t))^2 W_{t,j} W_{t,\Delta,j} f_t(S_t) f_t(S_t)^\top \right] \right]^{-1} \cdot E \left[\sum_{t=1}^T W_{t,j} W_{t,\Delta,j} \epsilon_{t,\Delta,j} (A_{t,j} - \tilde{p}_t(1 | S_t)) f_t(S_t) \times \sum_{t=1}^T W_{t,j} W_{t,\Delta,j} \epsilon_{t,\Delta,j} (A_{t,j} - \tilde{p}_t(1 | S_t)) f_t(S_t)^\top \right] \cdot \left[\sum_{t=1}^T E \left[(A_{t,j} - \tilde{p}_t(1 | S_t))^2 W_{t,j} W_{t,\Delta,j} f_t(S_t) f_t(S_t)^\top \right] \right]^{-1}$$

The outer terms are equal to $\left[\sum_{t=1}^T E \left[\tilde{p}_t(1 | S_t) (1 - \tilde{p}_t(1 | S_t)) f_t(S_t) f_t(S_t)^\top \right] \right]$, which gives us the covariance as desired.

We next consider asymptotic normality in the indirect setting. First, let

$$\epsilon_{t,\Delta,j} = Y_{t,\Delta,j} - g_t(H_t)^\top \alpha^{**} - (1 - A_{t,j})(A_{t,j} - \tilde{p}_t^*(1 | S_t)) f_t(S_t)^\top \beta^{**},$$

$\hat{\theta} = (\hat{\alpha}, \hat{\beta})$, and $\theta^{**} = (\alpha^{**}, \beta^{**})$. Since $S_t \subset H_t$ define

$h_{t,j}(H_t)^\top = (g_t(H_t)^\top, (1 - A_{t,j})(A_{t,j} - \tilde{p}_t^*(1 | S_t)) f_t(S_t)^\top)$. Then $\sqrt{M}(\hat{\theta} - \theta^{**})$ equals

$$\begin{aligned} & \sqrt{M} \left\{ \mathbb{P}_M \left(\frac{1}{G_m \cdot (G_m - 1)} \sum_{j=1}^{G_m} \sum_{j' \neq j} \sum_{t=1}^T W_{t,j,j'} W_{t,\Delta,j,j'} h_{t,j,j'}(H_t) h_{t,j,j'}(H_t)^\top \right)^{-1} \right. \\ & \left[\mathbb{P}_M \left(\frac{1}{G_m \cdot (G_m - 1)} \sum_{i=1}^{G_m} \sum_{j' \neq j} \sum_{t=1}^T W_{t,j,j'} W_{t,\Delta,j,j'} Y_{t,\Delta,j} h_{t,j,j'}(H_t) \right) \right. \\ & \left. - \mathbb{P}_M \left(\frac{1}{G_m \cdot (G_m - 1)} \sum_{j=1}^{G_m} \sum_{j' \neq j} \sum_{t=1}^T W_{t,j,j'} W_{t,\Delta,j,j'} h_{t,j,j'}(H_t) h_{t,j,j'}(H_t)^\top \right) \theta^{**} \right] \left. \right\} \\ & = \sqrt{M} \left[E \left[\frac{1}{G(G-1)} \sum_{j=1}^G \sum_{j' \neq j} \sum_{t=1}^T W_{t,j,j'} W_{t,\Delta,j,j'} h_{t,j,j'}(H_t) h_{t,j,j'}(H_t)^\top \right]^{-1} \right. \\ & \left. \left[\mathbb{P}_M \left(\frac{1}{G_m \cdot (G_m - 1)} \sum_{j=1}^{G_m} \sum_{j' \neq j} \sum_{t=1}^T W_{t,j,j'} W_{t,\Delta,j,j'} \epsilon_{t,\Delta,j,j'} h_{t,j,j'}(H_t) \right) \right] \right] + o_p(\mathbf{1}) \end{aligned}$$

By definitions of α^{**} and β^{**} and the previous consistency argument

$$E \left[\frac{1}{G \cdot (G-1)} \sum_{j=1}^G \sum_{j' \neq j} \sum_{t=1}^T W_{t,j,j'} W_{t,\Delta,j,j'} h_{t,j,j'}(H_t) h_{t,j,j'}(H_t)^\top \right] = 0$$

Then under moments conditions, we have asymptotic normality with variance Σ_θ given by

$$\begin{aligned} \Sigma_\theta &= E \left[\frac{1}{G \cdot (G-1)} \sum_{j=1}^G \sum_{j' \neq j}^G \sum_{t=1}^T W_{t,j,j'} W_{t,\Delta,j,j'} h_{t,j,j'}(H_t) h_{t,j,j'}(H_t)^\top \right]^{-1} \\ &\quad E \left[\frac{1}{G(G-1)} \sum_{j=1}^G \sum_{j' \neq j}^G \sum_{t=1}^T W_{t,j,j'} W_{t,\Delta,j,j'} \epsilon_{t,\Delta,j,j'} h_{t,j,j'}(H_t) \right. \\ &\quad \times \left. \frac{1}{G(G-1)} \sum_{j=1}^G \sum_{j' \neq j}^G \sum_{t=1}^T W_{t,j} W_{t,\Delta,j,j'} \epsilon_{t,\Delta,j,j'} h_{t,j,j'}(H_t)^\top \right] \\ &\quad E \left[\frac{1}{G \cdot (G-1)} \sum_{j=1}^G \sum_{j' \neq j}^G \sum_{t=1}^T W_{t,j,j'} W_{t,\Delta,j,j'} h_{t,j,j'}(H_t) h_{t,j,j'}(H_t)^\top \right]^{-1} \end{aligned}$$

Due to centering, the expectation of the matrix $W_{t,j,j'} h_{t,j,j'}(H_t) h_{t,j,j'}(H_t)^\top$ is block diagonal and the sub-covariance matrix Σ_β can be extracted and is equal to

$$\begin{aligned} \Sigma_\beta &= \left[\sum_{t=1}^T E \left[(1 - A_{t,j})(A_{t,j'} - \tilde{p}_t^*(1 | S_t))^2 W_{t,j,j'} W_{t,\Delta,j,j'} f_t(S_t) f_t(S_t)^\top \right] \right]^{-1} \\ &\quad \cdot E \left[\sum_{t=1}^T W_{t,j,j'} W_{t,\Delta,j,j'} \epsilon_{t,\Delta,j,j'} (1 - A_{t,j})(A_{t,j'} - \tilde{p}_t(1 | S_t)) f_t(S_t) \right. \\ &\quad \times \left. \sum_{t=1}^T W_{t,\tilde{j},\tilde{j}'} W_{t,\Delta,\tilde{j},\tilde{j}'} \epsilon_{t,\Delta,\tilde{j},\tilde{j}'} (1 - A_{t,\tilde{j}})(A_{t,\tilde{j}'} - \tilde{p}_t^*(1 | S_t)) f_t(S_t)^\top \right] \\ &\quad \cdot \left[\sum_{t=1}^T E \left[(1 - A_{t,j})(A_{t,j'} - \tilde{p}_t(1 | S_t))^2 W_{t,j,j'} W_{t,\Delta,j,j'} f_t(S_t) f_t(S_t)^\top \right] \right]^{-1} \end{aligned}$$

as desired.

Appendix C.: ADDITIONAL SIMULATION DETAILS

Appendix D.: SIMULATION FOR LAG EFFECT ESTIMATION

D.1. Simulation setup.

To evaluate the proposed estimator with $\Delta > 1$, we extend the simulation setup in the main paper. Consider an MRT with the same setting, in addition to $\beta_{\Delta 0} = -0.1$ and $\beta_{\Delta 1} = 0.2$, thus, $\Delta = 2$ and the proximal response is:

$$\begin{aligned} Y_{t,2} &= \theta_1 \{ S_{t+1} - E[S_{t+1} | A_t, H_t] \} + \{ A_t - p_t(1 | H_t) \} (\beta_{\Delta 0} + \beta_{\Delta 1} S_t) \\ &\quad + \{ A_{t+1} - p_{t+1}(1 | H_{t+1}) \} (\beta_{10} + \beta_{11} S_{t+1}) + e_{t+2}. \end{aligned} \tag{11}$$

Here we identify two prespecified future (after time t) "reference" treatment regimes that define the distribution for $A_{t+1}, \dots, A_{t+\Delta-1}$. The first one assigns treatment with probabilities between zero and one and corresponds to the treatment assignment distribution, and the second one chooses the reference regime $A_u = 1$ for $u > t$, with probability one. In this case, the lag Δ treatment effect represents the impact of a sequential treatments on the proximal response Δ time units later.

Simulation Scenario I.

The first scenario estimates β_{Δ}^* when an individual-level moderator exists and proximal responses share a random cluster-level intercept term that does not interact with treatment. The data generative model (11) incorporates a cluster-level random-intercept $e_g \sim \mathcal{N}(0, 0.5)$. Table 5 presents the results, which shows under both future treatment policies, the proposed C-WCLS approach achieve nearly unbiasedness and proper coverage.

Simulation Scenario II.

In the second scenario, we extend scenario I to include a random cluster-level intercept term that interacts with the treatment by considering the linear model with the additional term $b'_g \times (A_{t,j} - p_t(1 | H_{t,j}))$ where $b'_g \sim \mathcal{N}(0, 0.1)$. Table 5 presents the results which demonstrate that if cluster-level random effects interact with the previous treatment, then both policies produce nearly unbiased estimates and the proposed method achieves the nominal 95% coverage probability.

Simulation Scenario III.

In the third scenario, the lag treatment effect for an individual is assumed to depend on the average state of all individuals in the cluster, i.e., define the cluster-level moderator $\bar{S}_{t,g} = \frac{1}{G_g} \sum_{j=1}^{G_g} S_{t,j}$ and consider the linear model from Scenario II with the additional term $\bar{S}_{t,g} \times (A_{t,j} - p_t(1 | H_{t,j}))$. The proposed estimator again achieves the nominal 95% coverage probability (see Scenario III, Table 5).

D.2. Lag Treatment Effect Calculation. Sequential Treatment Regime.

As stated by the sequential treatment reference regime, we have the weight

$W_{t,\Delta} = \frac{\pi(A_{t+1} | H_{t+1})}{p(A_{t+1} | H_{t+1})} = \frac{1[A_{t+1} = 1]}{p(A_{t+1} | H_{t+1})}$. Thus, the true lag $\Delta = 2$ treatment effect can simply be calculated as:

$$\beta_{t,2} = E\left[Y_{t,2} \frac{1[A_{t+1} = 1]}{p(A_{t+1} | H_{t+1})} \mid H_t, A_t = 1\right] - E\left[Y_{t,2} \frac{1[A_{t+1} = 1]}{p(A_{t+1} | H_{t+1})} \mid H_t, A_t = 0\right] \quad (12)$$

Under our simulation setting, the term $E\left[Y_{t,2} \frac{1[A_{t+1} = 1]}{p(A_{t+1} | H_{t+1})} \mid H_t, A_t = a\right]$ is equal to:

$$\begin{aligned} & E[(0.8S_{t+1} + (A_t - p_t(1 | H_t))(-0.1 + 0.2S_t) + (A_{t+1} - p_{t+1}(1 | H_{t+1}))(-0.2 + 0.2S_{t+1})) \\ & \times \frac{1[A_{t+1} = 1]}{p(A_{t+1} | H_{t+1})} \mid H_t, A_t = a] \end{aligned}$$

Splitting the expectation above to three terms, we have the following calculation:

$$E\left[0.8S_{t+1} \frac{1[A_{t+1} = 1]}{p(A_{t+1} | H_{t+1})} \mid H_t, A_t = a\right] = 0 \quad (13)$$

$$\begin{aligned}
& E\left[(A_t - p_t(1 | H_t))(-0.1 + 0.2S_t) \frac{1[A_{t+1} = 1]}{p(A_{t+1} | H_{t+1})} \mid H_t, A_t = a\right] \\
&= (a - p_t(1 | H_t))(-0.1 + 0.2S_t) E\left[\frac{1[A_{t+1} = 1]}{p(A_{t+1} | H_{t+1})} \mid H_t, A_t = a\right] \\
&= (a - p_t(1 | H_t))(-0.1 + 0.2S_t)
\end{aligned} \tag{14}$$

$$\begin{aligned}
& E\left[(A_{t+1} - p_{t+1}(1 | H_{t+1}))(-0.2 + 0.2S_{t+1}) \frac{1[A_{t+1} = 1]}{p(A_{t+1} | H_{t+1})} \mid H_t, A_t = a\right] \\
&= E\left[(-0.2 + 0.2S_{t+1}) E\left[(A_{t+1} - p_{t+1}(1 | H_{t+1})) \frac{1[A_{t+1} = 1]}{p(A_{t+1} | H_{t+1})} \mid H_{t+1}\right] \mid H_t, A_t = a\right] \\
&= E\left[(-0.2 + 0.2S_{t+1})(1 - p_{t+1}(1 | H_{t+1})) \mid H_t, A_t = a\right] \\
&= -0.2 + 0.2 \cdot E[(1 - S_{t+1}) \cdot \text{expit}(-0.8A_t + 0.8S_{t+1}) \mid H_t, A_t = a] \\
&= -0.2 + 0.2 \cdot \text{expit}(-0.8a - 0.8)
\end{aligned} \tag{15}$$

Therefore,

$$\begin{aligned}
E\left[Y_{t,2} \frac{1[A_{t+1} = 1]}{p(A_{t+1} | H_{t+1})} \mid H_t, A_t = a\right] &= (13) + (14) + (15) \\
&= (a - p_t(1 | H_t))(-0.1 + 0.2S_t) - 0.2 + 0.2 \cdot \text{expit}(-0.8a - 0.8)
\end{aligned}$$

and the true lag $\Delta = 2$ treatment effect under sequential treatment regime is equal to:

$$\begin{aligned}
\beta_{t,2} &= E\left[Y_{t,2} \frac{1[A_{t+1} = 1]}{p(A_{t+1} | H_{t+1})} \mid H_t, A_t = 1\right] - E\left[Y_{t,2} \frac{1[A_{t+1} = 1]}{p(A_{t+1} | H_{t+1})} \mid H_t, A_t = 0\right] \\
&= -0.1 + 0.2S_t + 0.2 \cdot \text{expit}(-0.8 - 0.8) - 0.2 \cdot \text{expit}(-0.8) \\
&= -0.128 + 0.2S_t
\end{aligned} \tag{16}$$

Observed Distribution Treatment Regime.

As specified by this reference treatment regime, we have future treatment reference distribution the same with the distribution of treatments in the data we have at hand, i.e., $\pi(A_{t+1} | H_{t+1}) = p(A_{t+1} | H_{t+1})$ and $W_{t,\Delta} = 1$. Thus, the true lag $\Delta = 2$ treatment effect can be calculated as:

$$\beta'_{t,2} = E[Y_{t,2} \mid H_t, A_t = 1] - E[Y_{t,2} \mid H_t, A_t = 0] \tag{17}$$

Similar as above, under our simulation setting, the term $E[Y_{t,2} \mid H_t, A_t = a]$ is equal to:

$$\begin{aligned}
& E[(0.8S_{t+1} + (A_t - p_t(1 | H_t))(-0.1 + 0.2S_t) + (A_{t+1} - p_{t+1}(1 | H_{t+1}))(-0.2 + 0.2S_{t+1})) \mid H_t, A_t = a] \\
&= (18) + (19) + (20)
\end{aligned}$$

The three terms are calculated below:

$$E[0.8S_{t+1} \mid H_t, A_t = a] = 0 \tag{18}$$

$$E[(A_t - p_t(1 | H_t))(-0.1 + 0.2S_t) \mid H_t, A_t = a] = (a - p_t(1 | H_t))(-0.1 + 0.2S_t) \tag{19}$$

$$\begin{aligned}
& E[(A_{t+1} - p_{t+1}(1 | H_{t+1}))(-0.2 + 0.2S_{t+1}) | H_t, A_t = a] \\
&= E[(-0.2 + 0.2S_{t+1})E[(A_{t+1} - p_{t+1}(1 | H_{t+1})) | H_{t+1}] | H_t, A_t = a] \\
&= 0
\end{aligned} \tag{20}$$

Therefore,

$$E[Y_{t,2} | H_t, A_t = a] = (a - p_t(1 | H_t))(-0.1 + 0.2S_t)$$

and the true lag $\Delta = 2$ treatment effect under observed treatment distribution regime is equal to:

$$\begin{aligned}
\beta'_{t,2} &= E[Y_{t,2} | H_t, A_t = 1] - E[Y_{t,2} | H_t, A_t = 0] \\
&= -0.1 + 0.2S_t
\end{aligned} \tag{21}$$

D.3. Marginal Lag Treatment Effect Simulation Results.

The choice for prespecified future reference treatment regimes is of vital importance and often time yields to different treatment effect estimations. Following the derivations above, the fully marginal lag $\Delta = 2$ treatment effect is -0.128 for sequential treatment reference regime, and -0.1 for observed treatment distribution regime. Table 5 presents the simulation results.

Appendix E.: PROOF OF LEMMA 4.4

Proof.

Consider the W -matrix for the direct effect asymptotic variance,

$$\frac{1}{G^2} \sum_{t,t'} \sum_{j,j'} \mathbb{E} \left[W_{t,j} W_{t,\Delta,j} \epsilon_{t,\Delta,j} (A_{t,j} - \tilde{p}_t(1 | S_t)) W_{t',j'} W_{t',\Delta,j'} \epsilon_{t',\Delta,j'} (A_{t',j'} - \tilde{p}_t(1 | S_{t'})) f_t(S_t) f_{t'}(S_{t'})^\top \right]$$

Consider the cross-terms with $j \neq j'$ and without loss of generality assume $t \geq t'$, then

$$\begin{aligned}
& \mathbb{E} \left[\sum_{a,a'} \tilde{p}_t(a | S_t) (a - \tilde{p}_t(1 | S_t)) \tilde{p}_{t'}(a' | S_{t'}) (a' - \tilde{p}_{t'}(1 | S_{t'})) \right. \\
& \quad \left. \mathbb{E}[\mathbb{E}[W_{t,\Delta,j} \epsilon_{t,\Delta,j} W_{t',\Delta,j'} \epsilon_{t',\Delta,j'} | H_{t,j}, A_{t,j} = a, H_{t',j'}, A_{t',j'} = a'] | S_t, S_{t'}] f_t(S_t) f_{t'}(S_{t'})^\top \right].
\end{aligned}$$

Under the assumption of the error cross-term being constant in a and a' we can re-write the above as:

$$\begin{aligned}
&= \mathbb{E} \left[\sum_{a, a'} \tilde{p}_i(a | S_i)(a - \tilde{p}_i(1 | S_i))\tilde{p}_i(a' | S_i)(a' - \tilde{p}_i(1 | S_i))\psi(S_i, S_i)f_i(S_i)f_i(S_i)^\top \right] \\
&= \mathbb{E} \left[\psi(S_i, S_i)f_i(S_i)f_i(S_i)^\top \underbrace{\left(\sum_{a, a'} \tilde{p}_i(a | S_i)(a - \tilde{p}_i(1 | S_i))\tilde{p}_i(a' | S_i)(a' - \tilde{p}_i(1 | S_i)) \right)}_{=0} \right] \\
&= \mathbb{E} \left[\psi(S_i, S_i)f_i(S_i)f_i(S_i)^\top \cdot 0 \right] = 0.
\end{aligned}$$

Therefore, we have that the W -matrix simplifies to

$$\begin{aligned}
&\mathbb{E} \left[\sum_{t=1}^T W_{t,j}e_{t,j}(A_{t,j} - \tilde{p}_t(1 | S_t))f_t(S_t) \times \sum_{t=1}^T W_{t,j}e_{t,j}(A_{t,j} - \tilde{p}_t(1 | S_t))f_t(S_t)^\top \right] \\
&= \mathbb{E} \left[\frac{1}{G} \sum_{j=1}^G \left[\sum_{t=1}^T W_{t,j}e_{t,j}(A_{t,j} - \tilde{p}_t(1 | S_t))f_t(S_t) \times \sum_{t=1}^T W_{t,j}e_{t,j}(A_{t,j} - \tilde{p}_t(1 | S_t))f_t(S_t)^\top \right] \right] \\
&= \mathbb{E} \left[\sum_{t=1}^T W_{t,j}e_{t,j}(A_{t,j} - \tilde{p}_t(1 | S_t))f_t(S_t) \times \sum_{t=1}^T W_{t,j}e_{t,j}(A_{t,j} - \tilde{p}_t(1 | S_t))f_t(S_t)^\top \right]
\end{aligned}$$

which is the W matrix as in the standard MRT analysis. \square

Appendix F.: SMALL SAMPLE SIZE ADJUSTMENT FOR COVARIANCE ESTIMATION

The robust sandwich covariance estimator [24] for the entire variance matrix is given by $Q^{-1}\Lambda Q^{-1}$. The first term, Q , is given by

$$\sum_{m=1}^M \frac{1}{G_m} \sum_{j=1}^{G_m} D_{j,m}^\top W_{j,m} D_{j,m}$$

where $D_{j,m}$ is the model matrix for individual j in group g associated with equation (7), and $W_{j,m}$ is a diagonal matrix of individual weights. The middle term Λ is given by

$$\sum_{m=1}^M \frac{1}{G_m^2} \sum_{j=1}^{G_m} D_{j,m}^\top W_{j,m} (I_{i,m} - H_{i,m})^{-1} e_{i,m} e_{j,m}^\top (I_{j,m} - H_{j,m})^{-1} W_{j,m} D_{j,m}$$

where I_i is an identity matrix of correct dimension, e_i is the individual-specific residual vector and

$$H_{j,m} = D_{j,m} \left(\sum_{m=1}^M \frac{1}{G_m} \sum_{j=1}^{G_m} D_{j,m}^\top W_{j,m} D_{j,m} \right)^{-1} D_{j,m}^\top W_{j,m}$$

From $Q^{-1}\Lambda Q^{-1}$ we extract $\hat{\Sigma}_\rho$.

Appendix G.: ADDITIONAL ANALYSIS OF IHS

G.1. Additional Information for Figure 3.

Figure 3 presented a visually comparison between WCLS and C-WCLS in terms of the moderation of average previous week's proximal outcomes on the effect of notifications on average weekly mood scores, log step counts, and log sleep counts respectively in IHS. Here we attach the table for numerical comparison.

G.2. Lagged Treatment Effect.

We implement an extended investigation on the lag $\Delta = 2$ treatment effect of the targeted mobile notifications. The same two models: $\beta_2(t; S_t) = \beta_0 + \beta_1 \cdot Y_{t,j} + \beta_2 \bar{Y}_{t,-j}$ are applied to moderation analyses.

The first set of moderation analyses considers the standard moderation analysis where only individual-level moderators are included (i.e., $\beta_2 = 0$), with or without accounting for cluster-level moderation effect heterogeneity. Figure 4 and Figure 5 visualize the estimates across the range of prior week's proximal response for both our proposed approach and the WCLS approach from [3]. In this case, the effects do not change too much for all the analysis;

The second moderation analysis lets β_2 be a free parameter. Table 7 and Table 8 present the results. Here, we see that the constant term β_0 in the mood analysis becomes significant, while the new term β_2 is insignificant. The results suggest the average proximal outcomes of others in the cluster have a limited moderate effect on notifications, however, the lag impact of a notification on mood is positive and significant.

Appendix H.: ADDITIONAL DETAILS ON THE INDIRECT EFFECT

Weights used in the estimation of the indirect effect is a natural extension of [3]. As in Section 4.3, the weight $W_{t,j,j'}$ at decision time t for the j th individual is equal to $\frac{\tilde{p}(A_{t,j}, A_{t,j'} | S_t)}{p(A_{t,j}, A_{t,j'} | H_t)}$ where $\tilde{p}(a, a' | S_t) \in (0, 1)$ is arbitrary as long as it does not depend on terms in H_t other than S_t , and $p(A_{t,j}, A_{t,j'} | H_t)$ is the marginal probability that individuals j and j' receive treatments $A_{t,j}$ and $A_{t,j'}$ respectively given H_t .

In the simulation, the treatment individuals j and j' receive $A_{t,j}$ and $A_{t,j'}$ are mutually independent conditioning on the previous history. thus, the denominator of $W_{t,j,j'}$ can be factorized into:

$$p(A_{t,j}, A_{t,j'} | H_t) = p(A_{t,j} | H_t)p(A_{t,j'} | H_t)$$

Besides, the numerator of $W_{t,j,j'}$ is defined as the empirical frequency of the treatment pair (a, a') , which takes the value from $\{(0, 0), (0, 1), (1, 0), (1, 1)\}$. Here we denote it as

$$\tilde{p}_i(A_{i,j}, A_{i,j'} | S_i) = \hat{p}_i(A_{i,j}, A_{i,j'} | S_i)$$

Therefore, the weight we used in the simulation is constructed as:

$$W_{i,j,j'} = \frac{\hat{p}_i(A_{i,j}, A_{i,j'} | S_i)}{p(A_{i,j} | H_i)p(A_{i,j'} | H_i)}$$

When the numerators are estimated using the observed data, the variance-covariance must account for this. Throughout we allow for the setting in which individuals are not always available. For completeness we provide results for a more general estimating function which can be used with observational (non-randomized A_i) treatments, under the assumption of sequential ignorability and assuming the data analyst is able to correctly model and estimate the treatment probability $p(A_{i,j}, A_{i,j'} | H_i)$. We indicate how the results are simplified by use of data from an MRT.

Denote the parameterized treatment probability by $p_i(a, a' | H_i; \eta)$ (with parameter η); note η is known in an MRT. Denote the parameterized numerator of the weights by $\tilde{p}_i(a, a' | S_i; \rho)$ (with parameter ρ). The proof below allows the data analyst to use a \tilde{p}_i with an estimated parameter $\tilde{\rho}$ or to pre-specify ρ as desired. We use a superscript of \star to denote limiting values of estimated parameters (e.g. η^\star, ρ^\star). Then the more general version of the estimating equation $U_w(\alpha, \beta; \hat{\eta}, \hat{\rho})$ is:

$$\sum_{t=1}^T \left(Y_{t,1,j} - g_t(H_t) \right)^\top \alpha - (1 - A_{t,j})(A_{t,j'} - \tilde{p}_i^\star(1 | S_t; \hat{\rho})) f_t(S_t)^\top \beta \Big) I_{t,j} I_{t,j'} W_{t,j,j'}(A_{t,j}, A_{t,j'}, H_t; \hat{\eta}, \hat{\rho}) \times \begin{pmatrix} g_t(H_t) \\ (1 - A_{t,j})(A_{t,j'} - \tilde{p}_i^\star(1 | S_t; \hat{\rho})) f_t(S_t) \end{pmatrix}$$

Note $W_{t,j,j'}$ in the body of the paper is replaced here by $W_{t,j,j'}(A, H_t; \hat{\eta}, \hat{\rho})$, and $\hat{\eta}, \hat{\rho}$ are estimators.

Treatment Probability Model:

If the data is observational then we assume: $p_i(a, a' | H_i; \eta)$ is a correctly specified model for $\mathbb{P}(a, a' | H_i, I_{t,j} = 1, I_{t,j'} = 1)$. Let η^\star be the true value of η ; that is, $Pr(A_{t,j}, A_{t,j'} | H_i, I_{t,j} = 1, I_{t,j'} = 1) = p_i(a, a' | H_i; \eta^\star)$. Assume that the estimator of η , say $\hat{\eta}$, satisfies $\mathbb{P}_n U_D(\hat{\eta}) = 0$ and $\sqrt{n}(\hat{\eta} - \eta^\star) = \mathbb{E}[\dot{U}_D(\eta^\star)]^{-1} \mathbb{P}_n U_D(\eta^\star) + o_p(1)$. Thus $\sqrt{n}(\hat{\eta} - \eta^\star)$ converges in distribution to a mean zero, normal random vector with variance-covariance matrix given by $\mathbb{E}[\dot{U}_D(\eta^\star)]^{-1} \mathbb{E}[U_D(\eta^\star) \otimes U_D(\eta^\star)] \mathbb{E}[\dot{U}_D(\eta^\star)]^{-1}$, which has finite entries. Assume that $\mathbb{P}_n(\dot{U}_D(\hat{\eta}))$ is a consistent estimator of $\mathbb{E}(\dot{U}_D(\eta^\star))$. Assume there exists finite constants, $b_D > 0$ and $B_D < 1$ such that each $b_D < p_i(a, a' | H_i; \eta^\star) < B_D$ a.s.

If the data analyst elects to use a parameterized and estimated $\tilde{p}_i(1 | S_t, \hat{\rho})$, then we assume:

Numerator of Weights Probability Model:

Suppose the estimator $\hat{\rho}$ solves an estimating equation: $\mathbb{P}_n U_N(\rho) = 0$. Assume that, for a finite value of ρ , say ρ^* and $\sqrt{n}(\hat{\rho} - \rho^*) = \mathbb{E}[\dot{U}_N(\rho^*)]^{-1} \sqrt{n}(\mathbb{P}_n - P)U_N(\rho^*) + o_p(1)$ where the matrix, $\mathbb{E}[\dot{U}_N(\rho^*)]$ is positive definite. Assume $\sqrt{n}(\mathbb{P}_n - P)U_N(\rho^*)$ converges in distribution to a mean zero, normal random vector with variance-covariance matrix given by $\mathbb{E}[U_N(\rho^*)^{\otimes 2}]$ which has finite entries. Assume that $\mathbb{P}_n \dot{U}_N(\hat{\rho})$ is a consistent estimator of $\mathbb{E}[\dot{U}_N(\rho^*)]$. Assume $0 < \rho^* < 1$.

Proof.

The solution to $\mathbb{P}_n U_W(\alpha, \beta; \hat{\eta}, \hat{\rho}) = 0$ gives the estimator:

$$\begin{pmatrix} \hat{\alpha} \\ \hat{\beta} \end{pmatrix} = \{\mathbb{P}_n \dot{U}_W(\hat{\eta}, \hat{\rho})\}^{-1} \mathbb{P}_n \sum_{t=1}^T I_{t,J} I_{t,J} W_{t,J,J}(A_{t,J}, A_{t,J}, H_t; \hat{\eta}, \hat{\rho}) Y_{t,1,J} \times \begin{pmatrix} g_t(H_t) \\ (1 - A_{t,J})(A_{t,J} - \tilde{p}_t^*(1 | S_t))f_t(S_t) \end{pmatrix}$$

where

$$\dot{U}_W(\hat{\eta}, \hat{\rho}) = \sum_{t=1}^T I_{t,J} I_{t,J} W_{t,J,J}(A_{t,J}, A_{t,J}, H_t; \hat{\eta}, \hat{\rho}) \begin{pmatrix} g_t(H_t) \\ (1 - A_{t,J})(A_{t,J} - \tilde{p}_t^*(1 | S_t))f_t(S_t) \end{pmatrix}^{\otimes 2}$$

Define

$$\begin{pmatrix} \alpha' \\ \beta' \end{pmatrix} = \{\mathbb{E}[\dot{U}_W(\eta^*, \rho^*)]\}^{-1} \mathbb{E} \left[\sum_{t=1}^T I_{t,J} I_{t,J} W_{t,J,J}(A_{t,J}, A_{t,J}, H_t; \eta^*, \rho^*) Y_{t,1,J} \begin{pmatrix} g_t(H_t) \\ (1 - A_{t,J})(A_{t,J} - \tilde{p}_t^*(1 | S_t))f_t(S_t) \end{pmatrix} \right]$$

Then standard statistical arguments can be used to show that $\sqrt{n}(\hat{\alpha} - \alpha', \hat{\beta} - \beta')$ converges in distribution to a normal, mean zero, random vector with variance-covariance matrix given by:

$$\{\mathbb{E}[\dot{U}_W(\eta^*, \rho^*)]\}^{-1} \Sigma_W(\alpha', \beta'; \eta^*, \rho^*) \{\mathbb{E}[\dot{U}_W(\eta^*, \rho^*)]\}^{-1}$$

where

$$\Sigma_W(\alpha, \beta; \eta, \rho) = \mathbb{E} \left[\left(U_W(\alpha, \beta; \eta, \rho) + \Sigma_{W,D}(\alpha, \beta; \eta, \rho) \{\mathbb{E}[\dot{U}_D(\eta)]\}^{-1} U_D(\eta) + \Sigma_{W,N}(\alpha, \beta; \eta, \rho) \{\mathbb{E}[\dot{U}_N(\rho)]\}^{-1} U_N(\rho) \right)^{\otimes 2} \right]$$

with

$$\Sigma_{W,D}(\alpha, \beta; \eta, \rho) = \mathbb{E} \left[\sum_{t=1}^T \left(Y_{t,1,J} - g_t(H_t)^\top \alpha - (1 - A_{t,J})(A_{t,J} - \tilde{p}_t^*(1 | S_t; \rho)) f_t(S_t)^\top \beta \right) I_{t,J} I_{t,J} \right. \\ \left. W_{t,J,J}(A_{t,J}, A_{t,J}, H_t; \eta, \rho) \left(\begin{array}{c} g_t(H_t) \\ (1 - A_{t,J})(A_{t,J} - \tilde{p}_t^*(1 | S_t; \rho)) f_t(S_t) \end{array} \right) \left(\frac{d \log \tilde{p}_t^*(A_{t,J} | H_t; \eta)}{d \eta} \right)^\top \right],$$

and

$$\Sigma_{W,N}(\alpha, \beta; \eta, \rho) = \mathbb{E} \left[\sum_{t=1}^T \left(Y_{t,1,J} - g_t(H_t)^\top \alpha - (1 - A_{t,J})(A_{t,J} - \tilde{p}_t^*(1 | S_t; \rho)) f_t(S_t)^\top \beta \right) I_{t,J} I_{t,J} \right. \\ \left. W_{t,J,J}(A_{t,J}, A_{t,J}, H_t; \eta, \rho) \left(\begin{array}{c} g_t(H_t) \\ (1 - A_{t,J})(A_{t,J} - \tilde{p}_t^*(1 | S_t; \rho)) f_t(S_t) \end{array} \right) \left(\frac{d \log \tilde{p}_t^*(A_{t,J} | S_t; \rho)}{d \rho} \right)^\top \right] \\ + \mathbb{E} \left[\sum_{t=1}^T \left(Y_{t,1,J} - g_t(H_t)^\top \alpha - (1 - A_{t,J})(A_{t,J} - \tilde{p}_t^*(1 | S_t; \rho)) f_t(S_t)^\top \beta \right) I_{t,J} I_{t,J} \right. \\ \left. W_{t,J,J}(A_{t,J}, A_{t,J}, H_t; \eta, \rho) \left(\begin{array}{c} 0 \\ -(1 - A_{t,J}) \tilde{p}_t^*(1 | S_t; \rho) f_t(S_t) \end{array} \right) \left(\frac{d \log \tilde{p}_t^*(1 | S_t; \rho)}{d \rho} \right)^\top \right] \\ + \mathbb{E} \left[\sum_{t=1}^T (1 - A_{t,J}) \tilde{p}_t^*(1 | S_t; \rho) f_t(S_t)^\top \beta I_{t,J} I_{t,J} W_{t,J,J}(A_{t,J}, A_{t,J}, H_t; \eta, \rho) \right. \\ \left. \left(\begin{array}{c} g_t(H_t) \\ (1 - A_{t,J})(A_{t,J} - \tilde{p}_t^*(1 | S_t; \rho)) f_t(S_t) \end{array} \right) \left(\frac{d \log \tilde{p}_t^*(1 | S_t; \rho)}{d \rho} \right)^\top \right]$$

In our simulation, an individual's randomization probabilities only depends on their observed history, then $\tilde{p}_t^*(1 | S_{t,J}) = \tilde{p}_t^*(1 | S_t)$. Since the data is from an MRT (we know p_t) and we pre-specify (not estimate) \tilde{p}_t , then $\Sigma_w = \mathbb{E} \left[(U_w(\alpha, \beta)) \otimes^2 \right]$ greatly simplifying the variance-covariance matrix.

A consistent estimator of the variance-covariance matrix is given by:

$$\left\{ \mathbb{P}_n \left[\dot{U}_w(\hat{\eta}, \hat{\rho}) \right] \right\}^{-1} \hat{\Sigma}_w(\hat{\alpha}, \hat{\beta}; \hat{\eta}, \hat{\rho}) \left\{ \mathbb{P}_n \left[\dot{U}_w(\hat{\eta}, \hat{\rho}) \right] \right\}^{-1} \quad (22)$$

where

$$\hat{\Sigma}_w(\alpha, \beta; \eta, \rho) = \mathbb{P}_n \left[\left(U_w(\alpha, \beta; \eta, \rho) + \hat{\Sigma}_{W,D}(\alpha, \beta; \eta, \rho) \left\{ \mathbb{P}_n \left[\dot{U}_D(\eta) \right] \right\}^{-1} U_D(\eta) + \hat{\Sigma}_{W,N}(\alpha, \beta; \eta, \rho) \left\{ \mathbb{P}_n \left[\dot{U}_N(\rho) \right] \right\}^{-1} U_N(\rho) \right) \otimes^2 \right]$$

with

$$\hat{\Sigma}_{W,D}(\alpha, \beta; \eta, \rho) = \mathbb{P}_n \left[\sum_{t=1}^T \left(Y_{t,1,J} - g_t(H_t)^\top \alpha - (1 - A_{t,J})(A_{t,J} - \tilde{p}_t^*(1 | S_t; \rho)) f_t(S_t)^\top \beta \right) I_{t,J} I_{t,J} \right. \\ \left. W_{t,J,J}(A_{t,J}, H_t; \eta, \rho) \left(\begin{array}{c} g_t(H_t) \\ (1 - A_{t,J})(A_{t,J} - \tilde{p}_t^*(1 | S_t; \rho)) f_t(S_t) \end{array} \right) \left(\frac{d \log \tilde{p}_t^*(A_{t,J} | H_t; \eta)}{d \eta} \right)^\top \right],$$

and

$$\begin{aligned} \widehat{\Sigma}_{W,N}(\alpha, \beta; \eta, \rho) &= \mathbb{P}_n \left[\sum_{t=1}^T \left(Y_{t,1,J} - g_t(H_t) \right)^\top \alpha - (1 - A_{t,J})(A_{t,J} - \tilde{p}_t^*(1 | S_t; \rho)) f_t(S_t)^\top \beta \right) I_{t,J} I_{t,J} \\ &\quad W_{t,J,J}(A_{t,J}, A_{t,J}, H_t; \eta, \rho) \left(\begin{matrix} g_t(H_t) \\ (1 - A_{t,J})(A_{t,J} - \tilde{p}_t^*(1 | S_t; \rho)) f_t(S_t) \end{matrix} \right) \left(\frac{d \log \tilde{p}_t^*(A_{t,J} | S_t; \rho)}{d \rho} \right)^\top \right] \\ &+ \mathbb{P}_n \left[\sum_{t=1}^T \left(Y_{t,1,J} - g_t(H_t) \right)^\top \alpha - (1 - A_{t,J})(A_{t,J} - \tilde{p}_t^*(1 | S_t; \rho)) f_t(S_t)^\top \beta \right) I_{t,J} I_{t,J} \\ &\quad W_{t,J,J}(A_{t,J}, A_{t,J}, H_t; \eta, \rho) \left(\begin{matrix} 0 \\ -(1 - A_{t,J}) \tilde{p}_t^*(1 | S_t; \rho) f_t(S_t) \end{matrix} \right) \left(\frac{d \log \tilde{p}_t^*(1 | S_t; \rho)}{d \rho} \right)^\top \right] \\ &+ \mathbb{P}_n \left[\sum_{t=1}^T (1 - A_{t,J}) \tilde{p}_t^*(1 | S_t; \rho) f_t(S_t)^\top \beta I_{t,J} I_{t,J} W_{t,J,J}(A_{t,J}, A_{t,J}, H_t; \eta, \rho) \right. \\ &\quad \left. \left(\begin{matrix} g_t(H_t) \\ (1 - A_{t,J})(A_{t,J} - \tilde{p}_t^*(1 | S_t; \rho)) f_t(S_t) \end{matrix} \right) \left(\frac{d \log \tilde{p}_t^*(1 | S_t; \rho)}{d \rho} \right)^\top \right] \end{aligned}$$

It remains to show that $\beta' = \beta^* \star$. Since $\mathbb{E}[U_W(\alpha', \beta'; \eta^*, \rho^*)] = 0$,

$$0 = \mathbb{E} \sum_{t=1}^T \left(Y_{t,1,J} - g_t(H_t) \right)^\top \alpha' - (1 - A_{t,J})(A_{t,J} - \tilde{p}_t^*(1 | S_t; \rho^*)) f_t(S_t)^\top \beta' \Big) I_{t,J} I_{t,J}$$

$$\begin{aligned} &W_{t,J,J}(A_{t,J}, A_{t,J}, H_t; \eta^*, \rho^*) (1 - A_{t,J})(A_{t,J} - \tilde{p}_t^*(1 | S_t; \rho^*)) f_t(S_t) \\ &= \mathbb{E} \sum_{t=1}^T \left(\mathbb{E}[Y_{t,1} | A_{t,J}, A_{t,J}, H_t, I_{t,J} I_{t,J} = 1] - g_t(H_t) \right)^\top \alpha' - (1 - A_{t,J})(A_{t,J} - \tilde{p}_t^*(1 | S_t; \rho^*)) f_t(S_t)^\top \beta' \Big) \\ &I_{t,J} I_{t,J} W_{t,J,J}(A_{t,J}, A_{t,J}, H_t; \eta^*, \rho^*) (1 - A_{t,J})(A_{t,J} - \tilde{p}_t^*(1 | S_t; \rho^*)) f_t(S_t) \\ &= \mathbb{E} \sum_{t=1}^T \sum_{a' \in [0, 1]} \left(\mathbb{E}[Y_{t,1} | A_{t,J} = 0, A_{t,J} = a', H_t, I_{t,J} I_{t,J} = 1] - g_t(H_t) \right)^\top \alpha' - \\ &(a' - \tilde{p}_t^*(1 | S_t; \rho^*)) f_t(S_t)^\top \beta' \Big) I_{t,J} I_{t,J} \tilde{p}_t(0, a' | S_t; \rho^*) (a' - \tilde{p}_t^*(1 | S_t; \rho^*)) f_t(S_t) \end{aligned}$$

where the last equality averages out over $A_{t,J}$. The above simplifies to:

$$\begin{aligned} 0 &= \mathbb{E} \sum_{t=1}^T \sum_{a' \in \{0, 1\}} \left(\mathbb{E}[Y_{t,1} | A_{t,J} = 0, A_{t,J} = a', H_t, I_{t,J} I_{t,J} = 1] - g_t(H_t) \right)^\top \alpha' - \\ &(a' - \tilde{p}_t^*(1 | S_t; \rho^*)) f_t(S_t)^\top \beta' \Big) I_{t,J} I_{t,J} \tilde{p}_t(0, a' | S_t; \rho^*) (a' - \tilde{p}_t^*(1 | S_t; \rho^*)) f_t(S_t) \\ &= \mathbb{E} \sum_{t=1}^T \left(\mathbb{E}[Y_{t,1} | A_{t,J} = 0, A_{t,J} = 1, H_t, I_{t,J} I_{t,J} = 1] - g_t(H_t) \right)^\top \alpha' - \\ &(1 - \tilde{p}_t^*(1 | S_t; \rho^*)) f_t(S_t)^\top \beta' \Big) I_{t,J} I_{t,J} \tilde{p}_t(0, 1 | S_t; \rho^*) (1 - \tilde{p}_t^*(1 | S_t; \rho^*)) f_t(S_t) \\ &+ \mathbb{E} \sum_{t=1}^T \left(\mathbb{E}[Y_{t,1} | A_{t,J} = 0, A_{t,J} = 0, H_t, I_{t,J} I_{t,J} = 1] - g_t(H_t) \right)^\top \alpha' - \\ &(-\tilde{p}_t^*(1 | S_t; \rho^*)) f_t(S_t)^\top \beta' \Big) I_{t,J} I_{t,J} \tilde{p}_t(0, 0 | S_t; \rho^*) (-\tilde{p}_t^*(1 | S_t; \rho^*)) f_t(S_t) \\ &= \mathbb{E} \sum_{t=1}^T \left(\mathbb{E}[Y_{t,1} | A_{t,J} = 0, A_{t,J} = 1, H_t, I_{t,J} I_{t,J} = 1] - \mathbb{E}[Y_{t,1} | A_{t,J} = 0, A_{t,J} = 0, H_t, I_{t,J} I_{t,J} = 1] \right. \\ &\quad \left. - f_t(S_t)^\top \beta' \right) f_t(S_t) \gamma(\eta^*, \rho^*) I_{t,J} I_{t,J} \end{aligned}$$

where $\gamma(\eta^*, \rho^*) = \tilde{p}_i(0, 1 | S_i)(1 - \tilde{p}_i^*(1 | S_i; \rho^*)) = \tilde{p}_i(0, 0 | S_i)\tilde{p}_i^*(1 | S_i; \rho^*)$. From this we obtain:

$$0 = \mathbb{E} \sum_{t=1}^T f_i(S_t)\gamma(\eta^*, \rho^*)I_{t,J}I_{t,J'}(\mathbb{E}[\mathbb{E}[Y_{t,1} | A_{t,J} = 0, A_{t,J'} = 1, H_t, I_{t,J}I_{t,J'} = 1] - \mathbb{E}[Y_{t,1} | A_{t,J} = 0, A_{t,J'} = 0, H_t, I_{t,J}I_{t,J'} = 1] | S_t, I_{t,J}I_{t,J'} = 1] - f_i(S_t)^\top \beta')$$

Thus

$$\begin{aligned} \beta' &= [\mathbb{E}\dot{U}_w(\eta^*, \rho^*)]_{(2,2)}^{-1} \mathbb{E} \left[\sum_{t=1}^T f_i(S_t)\gamma(\eta^*, \rho^*)I_{t,J}I_{t,J'} \mathbb{E} \right. \\ & \left. [\mathbb{E}[Y_{t,1} | A_{t,J} = 0, A_{t,J'} = 1, H_t, I_{t,J}I_{t,J'} = 1] - \mathbb{E}[Y_{t,1} | A_{t,J} = 0, A_{t,J'} = 0, H_t, I_{t,J}I_{t,J'} = 1] | S_t, I_{t,J}I_{t,J'} = 1] \right] \end{aligned} \tag{23}$$

where

$$[\mathbb{E}\dot{U}_w(\eta^*, \rho^*)]_{(2,2)} = \mathbb{E} \sum_{t=1}^T f_i(S_t)f_i(S_t)^\top \gamma(\eta^*, \rho^*)I_{t,J}I_{t,J'}$$

□

Appendix I.: CONNECTION TO A SEMIPARAMETRIC EFFICIENT ESTIMATOR

A special case of both effects is when S_i is set to the observed history H_i and $\Delta = 1$. In this case, estimators for this fully conditional case can be derived using techniques from [25] based on semiparametric efficiency theory [26, 27] under a lack of interference assumption. Proofs can be found in Appendix I.1.

Lemma I.1.

Under the semiparametric model (4.1), Assumption 3.2, and the stronger lack of interference assumption, the semiparametric efficient score $S_{eff}(\beta)$ for β is

$$\frac{1}{G} \sum_{j=1}^G \sum_{t=1}^T \left(Y_{t,1,j} - \mu(H_{t,j}) - (A_{t,j} - p_i(1 | H_{t,j}))f_i(H_{t,j})^\top \beta \right) K_{i,j}(A_{t,j} - p_i(1 | H_{t,j}))f_i(H_{t,j}) \tag{24}$$

where

$$\begin{aligned} \mu(H_{t,j}) &= \mathbb{E}[Y_{t,1,j} | H_{t,j}], \quad \text{and} \quad \sigma_{i+1}^2(H_{t,j}, A_{t,j}) = \text{Var}(Y_{t,1,j} | H_{t,j}, A_{t,j}) \\ K_{i,j} &= \left[\frac{1}{\sigma_{i+1,j}^2(H_{t,j}, 1)} + p_i(1 | H_{t,j}) \left[\frac{p_i(1 | H_{t,j})}{\sigma_{i+1,j}^2(H_{t,j}, 1)} + \frac{1 - p_i(1 | H_{t,j})}{\sigma_{i+1,j}^2(H_{t,j}, 0)} \right] \right] \times \\ & \left(\frac{1}{\sigma_{i+1,j}^2(H_{t,j}, 1)} - \frac{1}{\sigma_{i+1,j}^2(H_{t,j}, 0)} \right). \end{aligned}$$

Semiparametric efficiency theory states that the solution $\hat{\beta}$ to $\mathbb{P}_n[S(\beta)] = 0$ achieves the semiparametric efficiency bound [26]. Corollary I.2 motivates the C-WCLS criterion

for the direct effect given by (7) from the semiparametric efficiency perspective under particular working homoskedastic assumptions on the conditional variance $\sigma_{t+1}^2(H_{t,j}, A_{t,j})$ and a working model $g(H_{t,j})^\top \alpha$ for the unknown quantity $\mu(H_{t,j})$. While this establishes a connection between the C-WCLS criterion and semiparametric efficiency scores, more work on efficiency theory for causal excursions effects is considered important future work.

Corollary I.2.

Assuming $\text{Var}(Y_{t+1,j} | H_{t,j}, A_{t,j}) = \sigma_{t+1}^2(H_{t,j})$, i.e., is constant in the second argument $A_{t,j}$, the weight $K_{t,j}$ is equal to $(\sigma_{t+1}^2(H_{t,j}))^{-1}$ and the semiparametric efficient score (24) weights each decision time by the corresponding conditional variance. Under the further assumption that this variance does not depend on the history, i.e., $\sigma_{t+1}^2(H_{t,j}) = \sigma^2$, and a working model for the conditional mean $\mu(H_{t,j}) = g(H_{t,j})^\top \alpha$, criterion (7) is equivalent to the semiparametric efficient score for the fully conditional effect.

I.1. Proof of semiparametric efficiency.

In this section, we assume lack of interference and therefore the potential outcomes can be written to only depend on one's observed history. Then we consider a semiparametric model characterized by the following assumptions:

Assumption I.3.

For all $t \leq T$, $E[Y_{t+1,j}(\bar{A}_{t-1,j}, 0) | H_{t,j}, A_{t,j}] = E[Y_{t+1,j}(\bar{A}_{t-1,j}, 0) | H_{t,j}]$

Assumption I.4.

Assume that there exists a function $\gamma(\cdot)$ and a true parameter $\psi_0 \in \mathbb{R}^p$, such that for any $1 \leq t \leq T$,

$$\mathbb{E}[Y_{t+1,j}(\bar{A}_{t-1,j}, a_t) | \bar{z}_t, \bar{a}_t] - \mathbb{E}[Y_{t+1,j}(\bar{A}_{t-1,j}, 0) | \bar{z}_t, \bar{a}_t] = \gamma(t+1, \bar{z}_t, \bar{a}_t; \psi)$$

We next gather the definitions necessary for defining the semiparametric efficient score:

1. The longitudinal data is $O_t, A_t, Y_{t,1}, Y_{t,2}, \dots, Y_{t,T}, A_t, Y_{t,1}$ where O_t is the time-varying covariates on all individuals in the cluster, A_t is the treatment assignments for the cluster, and $Y_{t,1}$ is the set of proximal outcomes on the cluster
2. $Z_{t,j} = (Y_{t,j}, O_{t,j})$
3. $H_{t,j} = (\bar{A}_{t-1,j}, \bar{Z}_{t,j})$
4. $V_{t,j} = (H_{t,j}, A_{t,j})$
5. $U_{t+1,j}(\psi) = Y_{t+1,j} - \gamma(t+1, \bar{z}_t, \bar{a}_t; \psi)$
6. $\dot{U}_{t+1,j}(\psi) = U_{t+1,j} - \mathbb{E}[U_{t+1,j} | H_{t,j}]$

$$7. \quad W_{t,j} = \text{Var}(U_{t+1,j}(\psi_0) | V_{t,j})^{-1}$$

Then by [4, Lemma I.8], a general form of the efficient score is

$$S_{\text{eff}}(\psi_0) = -\frac{1}{G} \sum_{j=1}^G \sum_{t=1}^T \rho_{t,j} \dot{U}_{t+1,j}(\psi_0)$$

where

$$\rho_{t,j} = \left[\mathbb{E} \left[\frac{\partial U_{t+1,j}}{\partial \psi} | V_{t,j} \right] - \mathbb{E} \left[\frac{\partial U_{t+1,j}}{\partial \psi} | H_{t,j} \right] \mathbb{E}(W_{t,j} | H_{t,j})^{-1} \right] W_{t,j}$$

Note that $\mathbb{E}[\rho_{t,j} | H_{t,j}] = 0$. Therefore by [4, Lemma I.1] we have

$$\rho_{t,j} = (\rho(A_{t,j} = 1) - \rho(A_{t,j} = 0))(A_{t,j} - p(1 | H_{t,j}))$$

where $\rho(A_{t,j} = a)$ denotes $\rho_{t,j}$ evaluated at $A_{t,j} = a$.

We now calculate these terms based on the above notation. Under

$\gamma(t+1, \bar{z}_t, \bar{a}_t; \psi_0) = A_{t,j} f(H_{t,j})^\top \psi$, we have

$$\frac{\partial U_{t+1,j}(\psi_0)}{\partial \psi} = -A_{t,j} f(H_{t,j}), \quad \text{and} \quad \dot{U}_{t+1,j}(\psi) = Y_{t+1,j} - \mu_t(H_{t,j}) + (A_{t,j} - p(1 | H_{t,j})) f_t(H_{t,j})^\top \psi$$

and hence we have

$$\mathbb{E} \left[\frac{\partial U_{t+1,j}(\psi_0)}{\partial \psi} | H_{t,j}, A_{t,j} = 1 \right] = -f(H_{t,j})$$

$$\mathbb{E} \left[\frac{\partial U_{t+1,j}(\psi_0)}{\partial \psi} | H_{t,j}, A_{t,j} = 0 \right] = 0$$

$$\text{Var}(U_{t+1,j}(\psi_0) | V_{t,j}) = \text{Var}(Y_{t+1,j} | V_{t,j}) =: \sigma_{t+1,j}^2(H_{t,j}, A_{t,j})$$

Then

$$\mathbb{E}[W_{t,j} | H_{t,j}] = \frac{p(1 | H_{t,j})}{\sigma_{t+1,j}^2(H_{t,j}, 1)} + \frac{1 - p(1 | H_{t,j})}{\sigma_{t+1,j}^2(H_{t,j}, 0)}$$

and we can express

$$\rho(A_{t,j} = 1) = - \left(1 - p(1 | H_{t,j}) \right) \left[\frac{p(1 | H_{t,j})}{\sigma_{t+1,j}^2(H_{t,j}, 1)} + \frac{1 - p(1 | H_{t,j})}{\sigma_{t+1,j}^2(H_{t,j}, 0)} \right] \frac{f(H_{t,j})}{\sigma_{t+1,j}^2(H_{t,j}, 1)}$$

$$\rho(A_{i,j} = 0) = - \left(0 - p(1 | H_{i,j}) \left[\frac{p(1 | H_{i,j})}{\sigma_{i+1,j}^2(H_{i,j}, 1)} + \frac{1 - p(1 | H_{i,j})}{\sigma_{i+1,j}^2(H_{i,j}, 0)} \right] \right) \frac{f(H_{i,j})}{\sigma_{i+1,j}^2(H_{i,j}, 1)}$$

Therefore $\rho_{i,j}$ is given by

$$\left[\frac{1}{\sigma_{i+1,j}^2(H_{i,j}, 1)} + p(1 | H_{i,j}) \left[\frac{p(1 | H_{i,j})}{\sigma_{i+1,j}^2(H_{i,j}, 1)} + \frac{1 - p(1 | H_{i,j})}{\sigma_{i+1,j}^2(H_{i,j}, 0)} \right] \right] \times$$

$$\left(\frac{1}{\sigma_{i+1,j}^2(H_{i,j}, 1)} - \frac{1}{\sigma_{i+1,j}^2(H_{i,j}, 0)} \right) \times (A_{i,j} - p(1 | H_{i,j})) f(H_{i,j}).$$

Moreover, under the simplifying assumption $\sigma_{i+1,j}^2(H_{i,j}, a) = \sigma_{i+1,j}^2(H_{i,j})$ we have

$$\rho_{i,j} = \frac{1}{\sigma_{i+1,j}^2(H_{i,j})} \times (A_{i,j} - p(1 | H_{i,j})) f(H_{i,j}).$$

Under the even stronger assumption $\sigma_{i+1,j}^2(H_{i,j}) = \sigma^2$ we have

$$S_{\text{eff}}(\psi_0) = \frac{\sigma^2}{G} \sum_{j=1}^G \sum_{t=1}^T \left(Y_{i,t,j} - \mu_t(H_{i,j}) - (A_{i,t,j} - p_t(1 | H_{i,t,j})) f_t(H_{i,t,j})^\top \beta \right) \times$$

$$\times (A_{i,t,j} - p_t(1 | H_{i,t,j})) f_t(H_{i,t,j}).$$

Appendix J.: CODE TO REPLICATE SIMULATION AND CASE STUDY RESULTS

The R code used to generate the simulation experiments and case study results in this paper can be obtained at <https://github.com/Herashi/MRT-mHealthModeration>.

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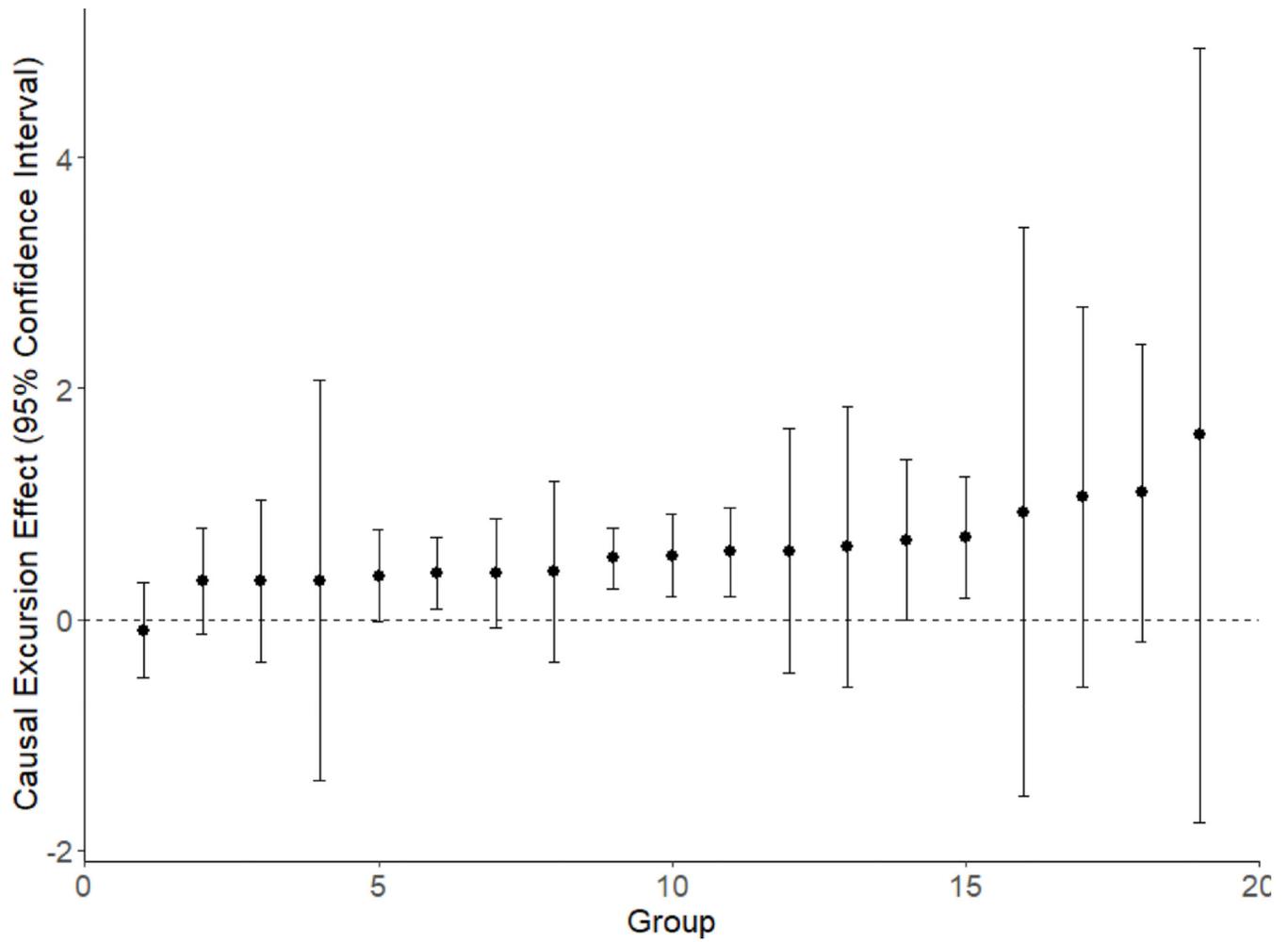


Figure 1. Heterogeneous estimated causal excursion effects across the largest $M=19$ clusters defined as specialties of size $G \geq 6$; the estimates are obtained using cluster-specific applications of the existing WCLS method.

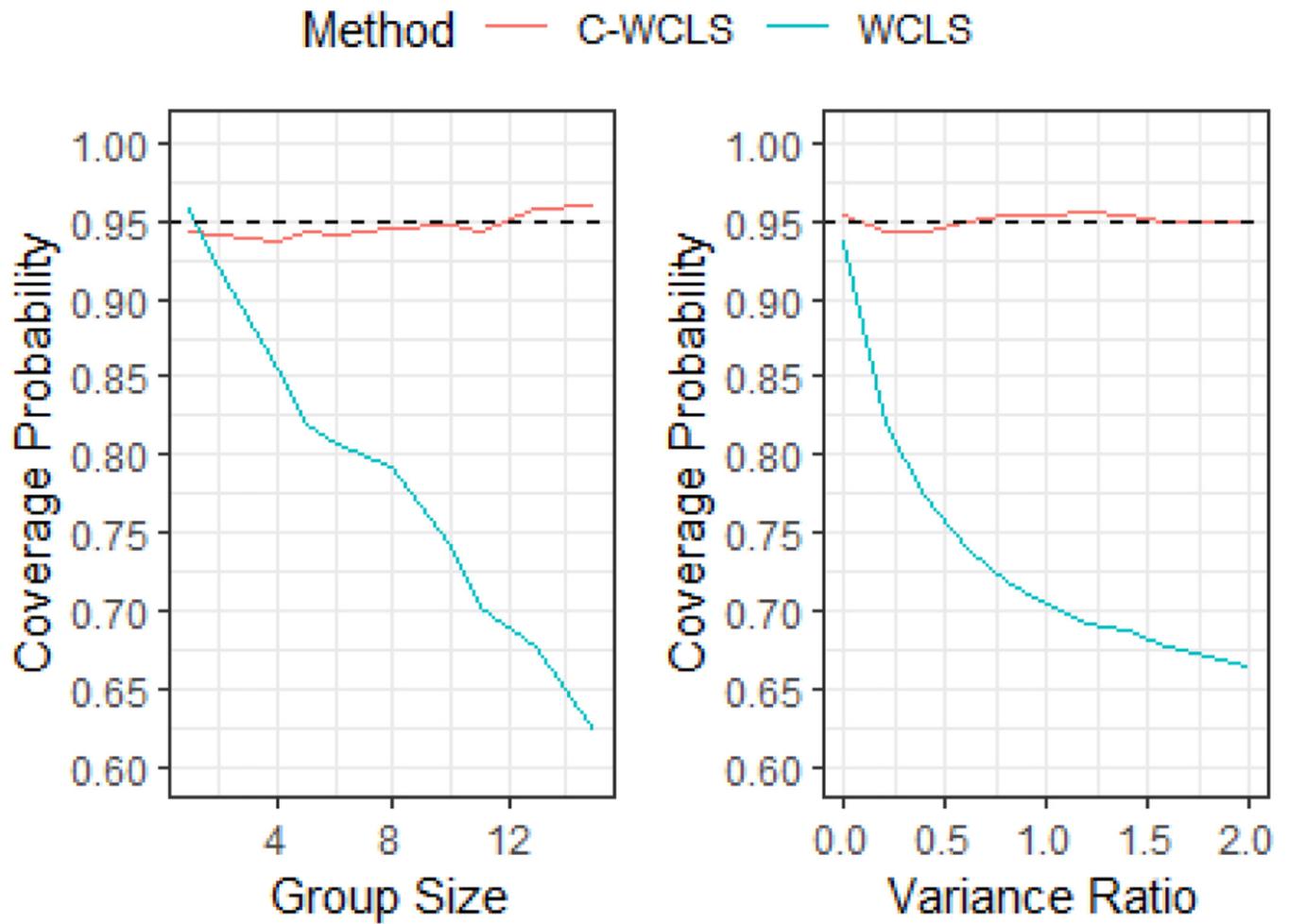


Figure 2. C-WCLS offers valid 95% confidence intervals in Scenario II. WCLS does not. Empirical coverage varies by group size (G) (**left**), and relative variance of b_g as compared to e_g (**right**).

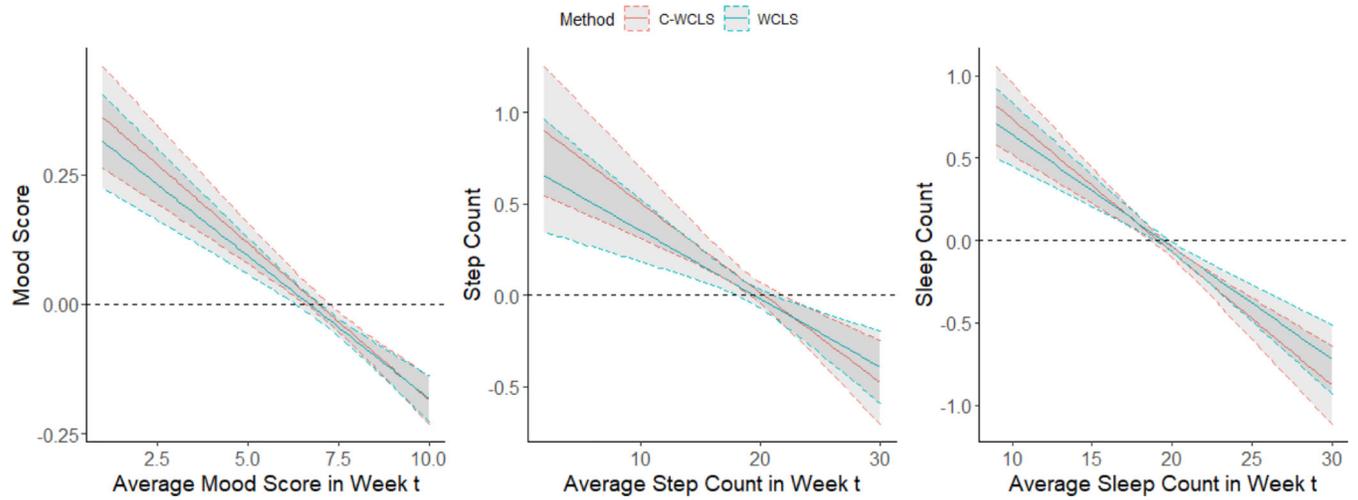


Figure 3. Moderation of average previous week's proximal responses on the effect of notifications on average weekly mood scores, log step counts, and log sleep counts respectively in IHS.

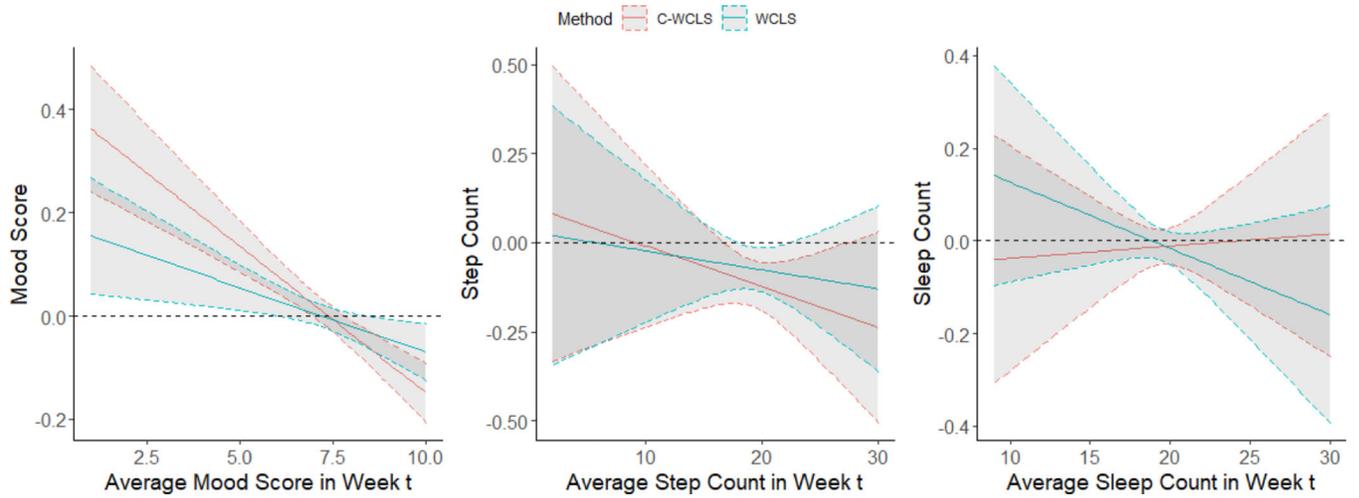


Figure 4. Moderation analysis of lag $\Delta = 2$ effect of notifications on average weekly mood scores, log step counts, and log sleep counts respectively under the sequential treatment policy.

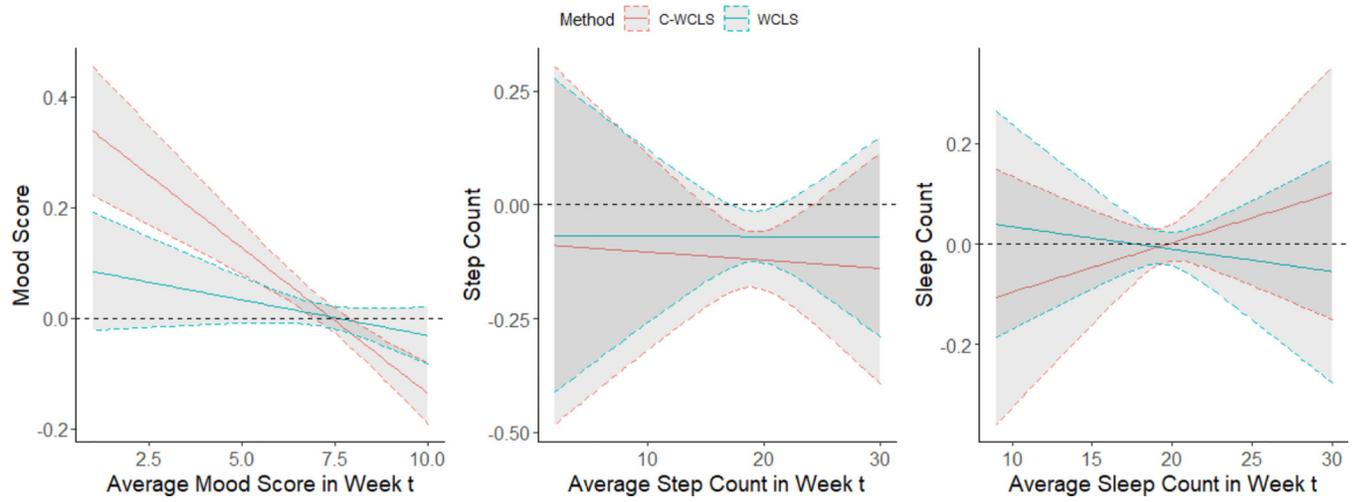


Figure 5. Moderation analysis of lag $\Delta = 2$ effect of notifications on average weekly mood scores, log step counts, and log sleep counts respectively under the observed treatment distribution.

Table 1.

Simulation: C-WCLS and WCLS comparison for Scenario I-IV.

Scenario	Estimator	# of Clusters	Cluster Size	Estimate	SE	RMSE	CP
I	C-WCLS	50	10	-0.198	0.025	0.027	0.935
	WCLS			-0.198	0.026	0.026	0.944
	C-WCLS	50	25	-0.198	0.016	0.016	0.950
	WCLS			-0.198	0.016	0.017	0.937
II	C-WCLS	50	10	-0.200	0.051	0.049	0.957
	WCLS			-0.200	0.029	0.052	0.723
	C-WCLS	50	25	-0.200	0.047	0.049	0.947
	WCLS			-0.199	0.019	0.048	0.555
III	C-WCLS	50	10	-0.198	0.051	0.052	0.941
	WCLS			-0.199	0.029	0.052	0.742
	C-WCLS	50	25	-0.199	0.047	0.048	0.946
	WCLS			-0.200	0.018	0.048	0.561
IV	C-WCLS	50	10	-0.097	0.020	0.021	0.953
			25	-0.100	0.013	0.013	0.942

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Table 2.

Moderation analysis for the direct and indirect effect of notifications on average weekly mood scores, log step counts, and log sleep minutes respectively in IHS. Coefficient $\tilde{\beta}_0$ represents the indirect effect under $A_{t,j} = 0$, while the coefficient $\tilde{\beta}_1$ represents the indirect effect under $A_{t,j} = 1$.

		Direct Effect			Indirect Effect			
	Variables	Estimate	Std. Error	p-value	Variables	Estimate	Std. Error	p-value
	Intercept (β_0)	0.563	0.251	0.028	$\tilde{\beta}_0$	-0.054	0.045	0.883
Mood	Prior Week Avg. (β_1)	-0.066	0.027	0.016	$\tilde{\beta}_1$	-0.015	0.031	0.684
	Cluster Pr. Wk. Avg. (β_2)	-0.016	0.017	0.349				
	Intercept (β_0)	1.165	0.782	0.139	$\tilde{\beta}_0$	-0.038	0.134	0.612
Steps	Prior Week Avg. (β_1)	-0.048	0.036	0.177	$\tilde{\beta}_1$	0.019	0.090	0.417
	Cluster Pr. Wk. Avg. (β_2)	-0.010	0.014	0.482				
	Intercept (β_0)	1.545	0.779	0.050	$\tilde{\beta}_0$	0.007	0.096	0.469
Sleep	Prior Week Avg. (β_1)	-0.081	0.039	0.037	$\tilde{\beta}_1$	-0.004	0.065	0.526
	Cluster Pr. Wk. Avg. (β_2)	0.000	0.006	0.961				

Table 3.

Additional simulation results: cluster-based weighted-centered least squares (C-WCLS) and weighted-least squares estimator (WCLS) comparison for Scenarios I, II, III, and IV.

Scenario	Estimator	# of Clusters	Cluster Size	Estimate	SE	RMSE	CP
I	C-WCLS	25	10	-0.198	0.035	0.036	0.945
	WCLS			-0.200	0.036	0.035	0.956
	C-WCLS	25	25	-0.199	0.022	0.023	0.948
	WCLS			-0.199	0.023	0.022	0.958
	C-WCLS	50	10	-0.198	0.025	0.027	0.935
	WCLS			-0.198	0.026	0.026	0.944
	C-WCLS	50	25	-0.198	0.016	0.016	0.950
	WCLS			-0.198	0.016	0.017	0.937
	C-WCLS	100	10	-0.199	0.018	0.018	0.949
	WCLS			-0.198	0.018	0.019	0.949
	C-WCLS	100	25	-0.198	0.011	0.012	0.941
	WCLS			-0.199	0.011	0.012	0.944
C-WCLS	25	10	-0.199	0.070	0.076	0.935	
WCLS			-0.201	0.041	0.076	0.710	
C-WCLS	25	25	-0.196	0.065	0.071	0.933	
WCLS			-0.200	0.026	0.065	0.557	
C-WCLS	50	10	-0.200	0.051	0.049	0.957	
WCLS			-0.200	0.029	0.052	0.723	
C-WCLS	50	25	-0.200	0.047	0.049	0.947	
WCLS			-0.199	0.019	0.048	0.555	
C-WCLS	100	10	-0.198	0.036	0.035	0.955	
WCLS			-0.198	0.021	0.037	0.718	
C-WCLS	100	25	-0.198	0.033	0.035	0.942	
WCLS			-0.199	0.013	0.032	0.583	
C-WCLS	25	10	-0.199	0.070	0.073	0.948	
WCLS			-0.202	0.041	0.074	0.734	
C-WCLS	25	25	-0.196	0.066	0.069	0.931	
WCLS			-0.200	0.026	0.068	0.563	
C-WCLS	50	10	-0.198	0.051	0.052	0.941	
WCLS			-0.199	0.029	0.052	0.742	
C-WCLS	50	25	-0.199	0.047	0.048	0.946	
WCLS			-0.200	0.018	0.048	0.561	
C-WCLS	100	10	-0.200	0.036	0.037	0.946	
WCLS			-0.200	0.021	0.037	0.740	
C-WCLS	100	25	-0.201	0.034	0.033	0.956	
WCLS			-0.198	0.013	0.034	0.555	

Table 4.

Simulations show strong finite sample estimation and accurate coverage for indirect effects.

Scenario	# of Clusters	Cluster Size	Estimate	SD	RMSE	CP
IV	25	10	-0.097	0.028	0.029	0.958
	25	25	-0.101	0.017	0.019	0.942
	50	10	-0.097	0.020	0.021	0.953
	50	25	-0.100	0.013	0.013	0.942
	100	10	-0.097	0.015	0.015	0.943
	100	25	-0.100	0.009	0.009	0.944

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Table 5.

Simulation: cluster-based weighted-centered least squares (C-WCLS) estimators for lag $\Delta = 2$ effect, under the policy of observed treatment distribution (OTD) versus sequential treatment (ST), and comparison for Scenarios I, II, III.

Scenario	Policy	# of Clusters	Cluster Size	Estimate	SE	RMSE	CP
I	OTD	50	10	-0.098	0.031	0.032	0.938
	ST			-0.123	0.062	0.063	0.949
	OTD	50	25	-0.098	0.020	0.020	0.948
	ST			-0.124	0.040	0.039	0.955
II	OTD	50	10	-0.099	0.054	0.054	0.944
	ST			-0.122	0.077	0.078	0.949
	OTD	50	25	-0.099	0.048	0.049	0.942
	ST			-0.121	0.059	0.061	0.950
III	OTD	50	10	-0.096	0.054	0.056	0.942
	ST			-0.122	0.075	0.075	0.948
	OTD	50	25	-0.099	0.048	0.050	0.944
	ST			-0.125	0.059	0.059	0.955

Table 6.Moderation Analysis with $\beta(t; S_i) = \beta_0 + \beta_1 \cdot Y_{i,j}$

Outcome	Setting	Variables	Estimate	Std. Error	t-value	p-value
Mood	WCLS	β_0	0.369	0.086	4.267	0.000
		β_1	-0.055	0.011	-4.822	0.000
	C-WCLS	β_0	0.421	0.214	1.968	0.053
		β_1	-0.061	0.028	-2.181	0.032
Steps	WCLS	β_0	0.729	0.295	2.472	0.015
		β_1	-0.037	0.015	-2.484	0.015
	C-WCLS	β_0	0.997	0.734	1.357	0.176
		β_1	-0.049	0.037	-1.343	0.181
Sleep	WCLS	β_0	1.325	0.350	3.782	0.000
		β_1	-0.068	0.017	-3.916	0.000
	C-WCLS	β_0	1.543	0.767	2.012	0.046
		β_1	-0.081	0.039	-2.082	0.039

Table 7.

Moderation analysis for lag $\Delta = 2$ treatment effect with cluster-level moderators, under the policy of sequential weeks of treatment

Outcome	Setting	Variables	Estimate	Std. Error	t-value	p-value
Mood	C-WCLS	β_0	0.665	0.321	2.072	0.040
		β_1	-0.067	0.037	-1.804	0.072
		β_2	-0.027	0.019	-1.393	0.164
Steps	C-WCLS	β_0	0.234	1.039	0.225	0.823
		β_1	-0.011	0.045	-0.254	0.800
		β_2	-0.007	0.021	-0.354	0.725
Sleep	C-WCLS	β_0	-0.073	0.887	-0.082	0.935
		β_1	0.002	0.043	0.049	0.961
		β_2	0.001	0.008	0.135	0.893

Table 8.

Moderation analysis for lag $\Delta = 2$ treatment effect with cluster-level moderators, under the policy of observed treatment distribution

Outcome	Setting	Variables	Estimate	Std. Error	t-value	p-value
		β_0	0.585	0.292	2.002	0.046
Mood	C-WCLS	β_1	-0.061	0.036	-1.702	0.090
		β_2	-0.022	0.021	-1.038	0.299
		β_0	0.107	0.951	0.113	0.911
Steps	C-WCLS	β_1	-0.001	0.041	-0.033	0.974
		β_2	-0.011	0.018	-0.629	0.531
		β_0	-0.211	0.802	-0.263	0.793
Sleep	C-WCLS	β_1	0.009	0.040	0.233	0.816
		β_2	0.001	0.007	0.193	0.848