Facultad de Ingeniería
Universidad de Concepción

UNIVERSIDAD DE CONCEPCIÓN
FACULTAD DE INGENIERÍA
DEPARTAMENTO DE INGENIERÍA INDUSTRIAL

EVIDENCE-DRIVEN SIMULATED DATA IN REINFORCEMENT LEARNING TRAINING FOR PERSONALIZED MHEALTH INTERVENTIONS

Tesis presentada para optar al grado de Magíster en Ingeniería Industrial

POR

Giorgio Stefano Ian Michele Galgano Cabrera

Profesor Guía
Juan Carlos Caro Seguel, Ph.D.

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Concepción (Chile)

Facultad de Ingeniería
Universidad de Concepción

UNIVERSIDAD DE CONCEPCIÓN
FACULTAD DE INGENIERÍA
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ABSTRACT

Physical inactivity remains one of the leading preventable causes of non-communicable chronic diseases and premature mortality worldwide. Digital health technologies offer scalable solutions to promote physical activity, yet their effectiveness depends on the system´s capability to adapt to users motivational and contextual states. Reinforcement learning (RL), particularly contextual bandit algorithms, provides a promising framework for such adaptive personalization. However, these algorithms face the cold start problem (CSP) which limits their initial performance due to the lack of user data. This study explores whether theory driven simulated data can mitigate the CSP in training RL systems for personalized physical activity recommendations.

A scoping review of empirical studies (included n = 18) on the Integrated Behavior Change model was conducted to extract population-level parameters describing controlled motivation, autonomous motivation, attitude, subjective norms, perceived behavioral control, intention and need for autonomy. These parameters informed the generation of a synthetic dataset, simulating 2,000 virtual users. An e-greedy algorithm was trained using this synthetic dataset and compared to its training in a real-world pilot conducted through the mHealth web-app *Apptivate* with 558 university students.

Results indicated strong alignment between synthetic and real behavioral patterns, with both reproducing the expected correlations among IBC constructs. The CB trained on synthetic data improved adherence predictions by approximately 12 percentage points over random allocation and demonstrated convergence patterns similar to those observed in real data. These findings suggest that behaviorally informed synthetic data can provide a feasible pre-training environment for adaptive algorithms, reducing dependency on early empirical data and preserving user privacy.

Integrating behavioral theory into synthetic data generation constitutes a practical and ethically sound strategy to address the cold start problem in personalized mobile health interventions. Our approach bridges psychological modeling and machine learning, enhancing interpretability, scalability, and the methodological transparency of digital behavior change systems.

Index

1. Introduction 5
2. Background 6
3. Theoretical Framework...8
4. Apptivate...10
5. Methods 13
5.1 Scoping Review...13
5.2 Simulation 14
5.3 Algorithm Training...15
5.4 Data analysis 16
6. Results 18
6.1 Literature Review 18
6.2 Simulated dataset 19
6.3 Pilot data...22
7. Discussion 26
8. Conclusion...28
References 29
Abbreviations...38
Supplemental Annex 39

Figure Index

Figure 1: Apptivate main menu and workout view (Source: Primary)............................11
Figure 2: Integrated behavioral change model (Source: Hegger et al. 2014)....................11
Figure 3: Prisma Flowchart 18
Figure 4: SEM fitted on simulated data...21
Figure 5: Transition matrix in difficulty assignment by cycle on simulated data 22
Figure 6: Estimated SEM from Pilot data...23
Figure 7. Completed days per user...24
Figure 8: Transition Matrix 25

Table Index

Table 1: Correlation Matrix of IBC constructs from Scoping Review............................19
Table 2: Simulated Sociodemographic attributes 20
Table 3: Pilot sociodemographic attributes 22

1. Introduction

Sedentarism remains one of the leading preventable causes of non-communicable chronic diseases and premature mortality worldwide (Saqib et al., 2020). Intervening this issue is a central goal of of modern day public health policies (World Health Organization, 2019). In this context, digital health technologies offer scalable solutions to promote physical activity, yet their effectiveness depends on the system´s capability to adapt to users motivational and contextual states. Reinforcement learning (RL), particularly contextual bandit algorithms, provides a promising framework for such adaptive personalization. However, these algorithms face the cold start problem which limits their performance due to the lack of initial data.

To address this limitation, an emerging question arises: Can theory-driven simulated data solve the cold start problem in training contextual bandits for personalized physical activity recommendations? The main objective is to evaluate the effectiveness of synthetic user data to mitigate the Cold Start Problem in contextual-bandit training for adaptive physical-activity recommendations. This study has three specific objectives:

1. Characterize physical-activity behavioral patterns among university students based on behavioral models via empirical meta-analysis.
2. To simulate synthetic user data from theory-driven parameters and train contextual bandit algorithms for personalized physical activity recommendations.
3. To experimentally validate and compare the effectiveness of contextual bandits trained on synthetic versus empirical user data in addressing the cold start problem.

The study aims to evaluate the effectiveness of synthetic user data in mitigating the cold start problem in contextual-bandit training for adaptive physical activity recommendations. To achieve this, the first step is to provide the theoretical and empirical background supporting our approach, followed by a scoping review to establish an empirical foundation for the IBC constructs. Based on these findings, a population of synthetic users will be simulated and used to train a reinforcement learning algorithm. Subsequently, a pilot study was conducted with real students from the Universidad de Concepción using Apptivate, a web application developed under the Fondecyt project "Tailored goals and individual choice: A field experiment on automated commitment devices for health behavior", which investigates the role of dynamic personalization and individual agency in promoting sustained physical activity (Caro et al., 2025). Finally, the algorithm's allocation of optimal training difficulty will be compared between models trained on synthetic versus real user data, to determine whether synthetic data can effectively replicate real behavioral patterns for training reinforcement learning algorithms in personalized physical activity interventions.

2. Background

The global burden of physical inactivity continues to pose a significant public health challenge, contributing to the rise in non-communicable diseases (NCDs) and premature mortality worldwide (Murray et al., 2019; World Health Organization, 2019). Physical activity beyond that needed for work or transportation, particularly exercise and sports played as leisure, is critical for optimal health. Digital health technologies have emerged as promising tools for promoting physical activity at scale, offering the potential to deliver personalized, context-aware interventions (Nahum-Shani et al., 2018). However, as with in-person interventions, the effectiveness of such technologies hinges on their ability to adapt in real time to individual users' behavioral patterns, motivational states, and contextual conditions that impact individual engagement (Gourlan et al., 2016; Vasconcellos et al., 2020). Reinforcement learning (RL) algorithms, particularly contextual bandits, offer a simple computational framework for such adaptive personalization (Lu et al., 2021). Deployment of such online personalization systems pose an initial training data challenge; how to ensure proper initial recommendations to users when little to any user data is initially available, a phenomenon known as the cold start problem (CSP) (Silva et al., 2023). Addressing this issue is especially critical in health behavior interventions, where early engagement is essential for sustained behavioral change.

Most common approaches to the CSP involve simulated data (or a combination of simulated and real data). Initial data simulation for recommendation systems in mobile health (mHealth) interventions differ from other common applications (e.g. marketing), because they are grounded in behavioral theories, thus a purely data-driven approach to initial data simulation is likely to fail. In this context, integrating behavioral theory into the generation of synthetic training data presents a novel and underexplored solution, one that bridges the gap between psychologically informed user modeling and data-driven personalization strategies.

Building upon this, recent simulation-based approaches have begun to consider introducing behavioral theories for the modeling of adaptive interventions. For example, (F. R. Cavallo & Toumazou, 2023) developed a recommender system grounded in the Behavior Change Wheel (BCW) and the COM-B model, which conceptualizes behavior (B) as an outcome of capability (C), opportunity (O), and motivation (M) (West & Michie, 2020). Their simulation integrates both behavioral and biological data such as physical activity history and leptin levels to dynamically adjust intervention content and difficulty. This illustrates how theory-informed simulations can enhance the plausibility and adaptiveness of artificial user environments.

Similarly, (Oetomo et al., 2023) proposed a simulation-based method that retrospectively modeled user interaction trajectories to enable pre-training of reinforcement learning agents (referred as warm-start). Their approach, informed by behavioral insights and empirical data, allowed agents to acquire plausible behavior patterns before deployment, offering a scalable alternative to traditional data collection. This retrospective simulation strategy is particularly pertinent in physical activity contexts, where real-world experimentation is logistically and ethically constrained. However, despite its advantages, this method remains largely reliant on past observational data for calibration, underlining the necessity of developing simulations that draw directly from validated behavioral theories.

As behavioral models such as COM-B provide increasingly accurate representations of human decision-making, reinforcement learning specifically through contextual bandit algorithms has emerged as a promising method to implement such insights in real-time adaptive systems. Contextual bandits (CB) extend the traditional multi-armed bandit framework by incorporating contextual information (e.g., user states, environmental conditions) to inform action selection, thus enabling personalized recommendations while balancing the exploration–exploitation trade-off (Athey et al., 2023). This computational efficiency is particularly suitable for behavior change settings, where rapid adaptation and individualized interventions are necessary.

Although empirical applications of CB have thus far concentrated on areas such as mental health or digital engagement, (Mohr et al., 2015) demonstrated their feasibility through non-contextual bandit algorithms that adaptively delivered motivational messages to promote physical activity among university students. While their study did not utilize contextual data, it highlights the potential of bandit-based decision systems in such behavioral interventions and points to the relevance of simulation as a testing ground for personalization strategies. A critical next step is the integration of contextual information and behavioral theory into contextual bandit initial feature set, particularly in the domain of physical activity, where such approaches remain underexplored.

More generally, the application of behavioral theories in synthetic data generation for training adaptive machine learning algorithms especially within reinforcement learning remains limited. Existing methods tend to rely on heuristic assumptions or statistical correlations, which may fail to reflect the complex interplay of psychological processes involved in behavior change, particularly in physical activity interventions. This study contributes to this emerging interdisciplinary field, evaluating an evidence-driven synthetic data approach to mitigate the CSP limitations in personalized physical activity recommendations using a theoretical framework for human behavior.

3. Theoretical Framework

The CSP is a central problem for initial algorithm training for online personalization systems (Oinas-Kukkonen et al., 2022; Sabiri et al., 2025). To mitigate the CSP limitations, researchers have increasingly adopted synthetic data and filtering methods (which rely on user profiling) to train adaptive algorithms before applying them in real-world contexts (Sabiri et al., 2025). User profiling could be helpful to address CSP but ultimately requires an initial user base for training, thus unsuitable for mHealth interventions, usually delivered at a smaller scale compared with recommendation systems for mobile applications. Synthetic data enables the simulation of user-item interactions under controlled parameters, allowing early-stage evaluation and tuning of personalization strategies.

Another solution is employing contextual bandit algorithms (Pilani et al., 2021), in particular methods based on upper confidence bound (UCB), on both synthetic and real datasets, demonstrating that synthetic environments can support effective parameter learning and improve model performance. Notably, these algorithms, trained on simulated user profiles, achieved significantly lower cumulative regret when tested on large-scale datasets such as LastFM and MovieLens20M. These findings reinforce the utility of synthetic data in initializing personalized recommendation systems. However, such frameworks are typically constructed using structural or statistical rules, which may not adequately reflect the motivational, cognitive, and contextual dimensions that shape health-related behavior, particularly in physical activity interventions.

While rule-based generated synthetic datasets provide scalability and technical validation, they often fail to capture the psychological fidelity required for modeling user behavior change. Most synthetic frameworks abstract user behavior through feature distributions or clustering techniques without modeling underlying determinants such as intention formation, self-efficacy, or perceived control (Cane et al., 2012). In contrast, theory-driven simulations grounded in socio-cognitive models like the IBC or COM-B offer a richer account of user behavior by explicitly incorporating motivational dynamics and stage transitions. These models enable the simulation of users who exhibit temporally coherent and context-sensitive patterns of action, which are critical for training algorithms intended for behavior change applications (Park et al., 2023). Nevertheless, the integration of such theory-driven approaches into synthetic data generation remains limited within the machine learning community, particularly in reinforcement learning. Bridging this gap is essential for developing adaptive systems that are both technically robust and psychologically informed.

The reviewed literature reveals several important limitations. First, although synthetic data can lower implementation costs and improve algorithm training, most current approaches do not account for the cognitive and motivational complexity of real users. Second, the application of behavioral theory, especially the IBC model, in the design of training data for reinforcement learning systems remains scarce. Third, while contextual bandits show promise for personalized intervention delivery, their use in the domain of physical activity is still limited. To the best of our knowledge, no prior study has validated whether synthetic populations generated from socio-cognitive models can effectively address the cold start problem in this specific context.

While several models have been studied for physical activity as a behavior, the Integrated Behavioral Change (IBC) model is a better fit for this study. The IBC proposes a phase-based socio-cognitive framework for understanding physical activity as a behavior (Hagger & Chatzisarantis, 2014). It delineates three stages: pre-motivational (awareness), motivational, and post-motivational (action), each influenced by specific determinants such as cognizance, risk perception, attitude, social norms, and self-efficacy.

In contrast to models like the Theory of Planned Behavior (TPB), the IBC model explicitly incorporates distal variables (e.g., knowledge, cues to action, contextual factors) and considers both implicit and explicit cognitive processes (Ajzen, 1991). According to Cheung et al. (2020), the IBC model effectively captures the pathways from awareness to intention and behavior in the context of physical activity and may outperform other frameworks in intervention design due to its conceptual integration and explanatory depth. Furthermore, its incorporation of constructs from Self-Determination Theory (SDT) underscores the influence of cognitive factors such as attitude and perceived competence on motivational processes, although SDT variables alone did not significantly predict behavior in their longitudinal analysis (Vasconcellos et al., 2020).

4. Apptivate

For this project, the experiment was conducted using the web-app "Apptivate" (Cárcamo-Regla et al., 2024) (https://goals.apptivate.cl), extending its initial functionally to incorporate contextual bandit algorithms connected to a routine difficulty assignment. Apptivate creates workout routines with three different difficulty levels, changing the total workout duration as well as rest times between exercises. Physical activity professionals validated the routine design, ensuring that workouts match recommended guidelines for healthy adults. The overall design allows users to conduct exercises without equipment, following the in-app instructions, covering different muscle groups, as well as providing both warm-up and stretching exercises (Figure 1).

Apptivate adopts an adapted version of the IBC Model for physical activity (Hagger & Chatzisarantis, 2014) as a framework for tailoring workout difficulty recommendations, along with behavioral characteristics (traditional IBC model shown in Figure 2). We extended the IBC model to include need for autonomy and controlled motivation. The adapted IBC model constructs are defined as: autonomous motivation (AM); refers to the individual's intrinsic interest in the activity, attitude (ATT); is the person's perception regarding completing the activity, subjective norm (SN); represents the alignment with the interests or expectations of others, perceived behavioral control (PBC); is the perception that the necessary conditions exist to complete the activity, intention (INT); reflects the individual's willingness or readiness to perform the activity, need for autonomy (NFA); is the perception of self-determination in carrying out the activity, controlled motivation (CM); refers to the extent to which motivation originates from external sources. Solid arrows in the model denote core, empirically supported causal relationships, whereas dashed arrows indicate secondary or moderating pathways. By leveraging the IBC model, the app ensures that its recommendations address not only dynamic changes in behavior over time but also the psychological factors that influence behavior change. The application combines a user-friendly interface with adaptive features that respond to user preferences and contextual variables, aiming to create a more engaging and personalized experience. Among its main design components are dynamic notifications, motivational messages, progress visualization, and customization elements intended to increase perceived relevance and commitment. The app was developed as part of the Fondecyt project "Tailored goals and individual choice: A field experiment on automated commitment devices for health behavior", which investigates the role of dynamic personalization and individual agency in promoting sustained physical activity (Caro et al., 2025).

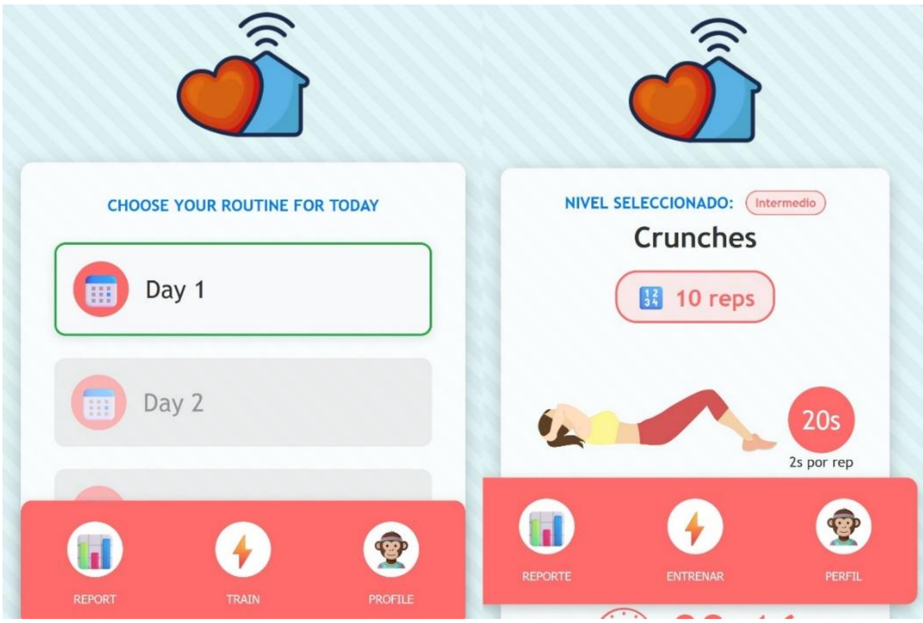


Figure 1: Apptivate main menu and workout view (Source: Primary).

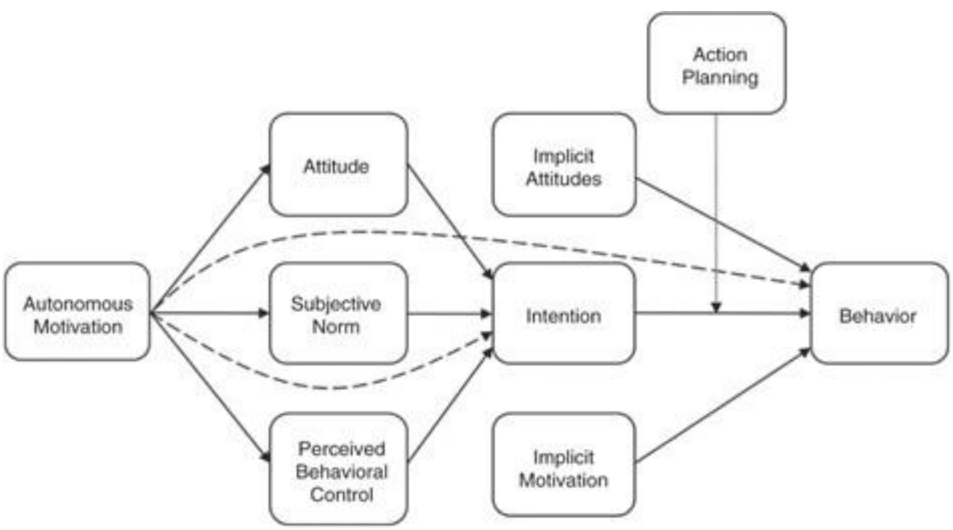


Figure 2: Integrated behavioral change model (Source: Hegger et al. 2014)

The pilot intervention had a duration of seven consecutive days, divided into two three-day training cycles with one rest day in between. The scope of this pilot are primarily university students and young adults, recruited through digital channels and social media campaigns.

Upon registration, participants complete a short questionnaire that provided baseline data on demographic characteristics, exercise habits, and motivational orientation. Based on this information, each user was assigned to a difficulty level (easy, moderate, or difficult) at random. After completing the first cycle (random), the algorithm was trained to provide a recommendation for the second cycle (optimal). Throughout the intervention, the system continuously logged user interactions with the app, including daily logins, routine completions, and engagement with personalization features such as schedule selection or avatar customization.

In addition to behavioral data, a qualitative post-intervention survey was conducted to assess user satisfaction, perceived utility, and motivational impact of the implemented personalization features. The instrument combined Likert-scale questions and open-ended items, allowing the collection of both quantitative indicators and qualitative insights into the user experience. A satisfaction threshold of four out of five was considered acceptable for each feature, while at least seventy percent positive responses were used as a benchmark for validation.

The data structure of the pilot was designed to enable detailed behavioral tracking and subsequent statistical analysis. Each user action was recorded with a time stamp and stored in the system database, ensuring traceability across the different features. Core variables included the number of completed routines, use of the avatar function, activation of the scheduling feature, reception of reminder messages, and daily app access.

5. Methods

5.1 Scoping Review

A scoping review was conducted to identify empirical studies examining behavioral determinants of physical activity within the IBC model. The search was performed in the Europe PMC database, encompassing publications from 2005 to 2024, as this period includes the main empirical applications of the IBC framework to health behavior research. Only peer-reviewed empirical studies available in full text and written in English were considered. The search string was designed to identify studies focusing on physical activity and the motivational constructs derived from the Self-Determination Theory and the Theory of Planned Behavior, including the terms “physical activity” or “exercise” combined with “self-determination theory” or “theory of planned behavior,” and “university students,” “students,” or “adults.” The final search query was:

> (TITLE_ABS:(((physical activity) OR (exercise)) AND ((self-determination theory) OR (theory of planned behavior)) AND ((university students) OR (students) OR (adults))) OR KEYWORD:(((physical activity) OR (exercise)) AND ((self-determination theory) OR (theory of planned behavior)) AND ((university students) OR (students) OR (healthy adults)))) AND (FIRST_PDATE:[2005 TO 2024]) AND (HAS_FT:Y OR (HAS_FREE_FULLTEXT:Y)) AND (((SRC:MED OR SRC:PMC OR SRC:AGR OR SRC:CBA) NOT (PUB_TYPE:"Review")))

Studies were eligible if they included healthy participants aged between 18 and 29 years, and if they quantitatively assessed at least one psychological construct aligned with the IBC model. To ensure theoretical consistency, studies had to employ validated instruments such as the Behavioral Regulation in Exercise Questionnaire (BREQ-2 or BREQ-3) or the Godin–Shephard Leisure-Time Physical Activity Questionnaire (GSLTPAQ). Additionally, studies were required to report descriptive statistics and/or correlation coefficients between IBC variables to enable quantitative synthesis. Only empirical quantitative studies published in peer-reviewed journals were considered, while review papers, theoretical articles, and studies on clinical or athletic populations were excluded. Data will be extracted following PRISMA-ScR guidelines, including study characteristics, measurement tools, and descriptive and correlational statistics. The extracted values will be standardized and integrated into a generalized correlation matrix to inform the parameter structure for subsequent simulation modeling.

5.2 Simulation

Based on the average estimates from empirical studies reviewed, a model was constructed to simulate the IBC constructs for a synthetic population using a multivariate joint distribution (Johnson, 1987; Niu & Hoff, 2019). To ensure the data matches with the empirical results, additional skewness was introduced in the model, as often occurs in ordered categorical self-reported data (Klein & Doll, 2021). As such, given mean values (μ) and covariance matrix (Σ), the vector of simulated IBC constructs for each individual "i" was generated as:

$$IBC_i = \mu + z_i L + s_i$$

Where z_i is a vector generated randomly from a standardized multinomial distribution and L is a lower triangle matrix such that $LL' = \Sigma$ (Cholesky decomposition). In order to introduce skewness, we propose a variant of the results for simulation discussed in Ghorbanzadeh (2014). We define the skewness factor (s_i) as:

$$s_i = \mathbf{1}\{u_i > 0\}(\delta * | v_i |)$$

Where $\delta = \frac{\alpha}{\sqrt{1+\alpha'\alpha}}$ is a scaling factor with α is a vector with values drawn from an independent uniform distribution [-2,2), and both u_i and v_i are vectors generated randomly from a standardized multinomial distribution.

The simulated agents reproduced the empirical data observed among IBC variables and incorporates sociodemographic features representative of the distribution of university students in a high-income country. To simulate sociodemographic features (gender, income, current physical activity), the mean and distribution values were extracted from the literature review and adapted to the Apptivate pilot context when necessary. To ensure statistical feasibility given the data available from the literature review, Σ was adjusted to ensure positive semi definiteness by adding $\epsilon = 0.00001$ to the smallest eigenvalue.

Once synthetic user data is generated, a process is required to determine behavioral adherence (i.e. goal competition) without any prior information. As noted in prior studies, we propose a continuous function mapping that assigns value to a non-linear combination of the simulated constructs and sociodemographic data, giving a score that represents the likelihood of adherence to behavior (Bierlaire, 1998). We used the IBC constructs, gender, income and current exercise in linear interactions with (the randomly) allocated difficulty levels, using the covariance matrix as reference weights, reporting a continuous value for each individual. Reference weights include differences in behavior adherence by individual characteristics, as well as correlations between IBC constructs and reported behavior, if available in the reported studies. As observed in the previous empirical literature, three aspects characterize the mapping function in relation to behavior adherence for physical activity: (1) women report lower adherence rates, (2) income is related to higher adherence, and (3) current physical activity is linked to higher adherence (Bergman et al., 2008).

In order to compare with the real data, each agent's simulated continuous value was mapped to a binary outcome for the cycle (success = 1), using percentile thresholds for each difficulty level fitting a mean adherence of 50%, as observed in previous literature (Peters et al., 2023). The function yielded by construction a decreasing gradient between adherence and difficulty level.

5.3 Algorithm Training

The resulting synthetic dataset was used to train an online contextual bandit algorithm setting, in particular epsilon greedy (ε-greedy) (Cortes, 2019). The contextual bandits model learns to personalize goal difficulty (1: easy, 2: moderate, or 3: difficult) based on user context, optimizing adherence as the reward signal. Each simulated and real participant was initially randomized to one of the three difficulty groups with equal probability, establishing a logging policy for the first cycle.

During training, the model implemented a ε-greedy exploration strategy to balance exploration and exploitation in the learning process. With probability ε (set at 0.2), the algorithm randomly selected an action to promote exploration and prevent overfitting to early experiences. With the complementary probability (1−ε), it exploited its current knowledge by choosing the action with the highest estimated reward according to the learned policy. Each interaction was represented as an action-dependent feature (ADF) example combining static psychological variables (e.g., autonomous motivation, attitude, subjective norm, perceived behavioral control, intention) and contextual states that modulated behavior dynamically. After each simulated episode, the policy parameters were updated online using stochastic gradient descent, minimizing the expected cost weighted by the probability of action selection. Through this iteration, the contextual bandit progressively improved its capacity to predict and recommend goal difficulty levels that maximize adherence, approximating a personalized and adaptive decision-making system grounded in behavioral theory. As shown in the following pseudocode:

Epsilon-greedy
Inputs:
$\varepsilon = 0.2$ and decay rate $\mathrm{d} = 0.01$
$x = user\ context\ (IBC\ constructs\ and\ sociodemographic\ data)$
$\alpha \in \mathrm{k} = \{1, 2,3\}\ (action\ set: 1 - easy, 2 - medium, 3 - hard)$
$binary\ reward\ r \epsilon \{0,1\}$
$\hat{f}_k =$ mapping funtcion $of\ rewards\ for\ action\ k\ given\ a\ context\ x$

for each succesive round t with context $x^t\ do$:
$With\ probability\ (1 - \varepsilon)$
$Select\ action\ \alpha = argmax_k \hat{f}_k(x^t)$
$Otherwise$:
$Select\ action\ \alpha\ uniformly\ at\ random\ from\ 1\ to\ k$
$Obtain\ reward\ r_a^t, Update\ \{x^t, r_a^t\}$
$Update\ \hat{f}_a\ and\ \varepsilon = \mathrm{d} * \varepsilon$
End

5.4 Data analysis

A comparative analysis was carried out to explore the performance of contextual bandit algorithms trained on empirically calibrated synthetic versus real user data (from the Apptivate pilot study). This comparison seeks to examine the extent to which behavioral patterns and adherence dynamics generated in the simulated environment align with those observed in real participants under similar experimental conditions. To contrast the simulated versus real IBC model constructs, structural equation models (SEM) were applied to the baseline questionnaire in the real dataset and using the simulated data (Bollen & Davis, 2009) following the validated structure described in the study protocol (Caro et al., 2025). In particular, the fitted model has the following structure (using the adapted IBC model notation):

$$INT \sim AM + PBC + SN + ATT + CM$$
$$SN \sim AM + CM$$
$$PBC \sim AM + CM$$
$$CM \sim NFA + AM$$
$$AM \sim NFA + CM$$

In each case, the estimated model is reported (coefficient and p-value), as well as relevant fit indices; Goodness-of-Fit, GFI (ranged between 0 and 1) and Root Mean Squared Error of Approximation (RMSEA). Additionally, for both real and simulated conditions, average adherence rates and transition matrices were computed to compare difficulty level assignment between random to optimal allocation across cycles.

6. Results

6.1 Literature Review

The initial search identified 215 records. Titles and abstracts were screened to remove duplicates and exclude studies that did not meet the theoretical or population criteria. The remaining articles were evaluated in full text to confirm the presence of relevant constructs and extract the necessary data. After applying the inclusion and exclusion criteria, 18 studies were retained for the final synthesis. From these studies, data were extracted regarding authorship, year of publication, sample size, country, participant characteristics, instruments used, and statistical information including means, standard deviations, and correlations among IBC constructs. All data were standardized to ensure comparability across studies. The overall description of the studies in the literature review can be found in Table A1 and the PRISMA flowchart summarizing the scoping review can be found in Figure 3.

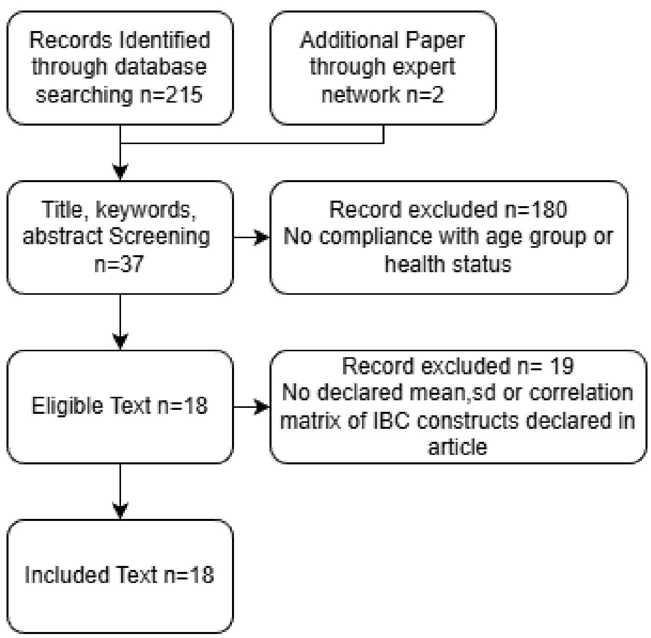


Figure 3: Prisma Flowchart

The information collected from the included studies was used to construct a generalized correlation matrix that summarized the interrelations among the principal IBC constructs in Table 1. This matrix served as the empirical foundation for developing the covariance structure used in the subsequent simulation phase. The resulting data showed a high degree of theoretical and empirical coherence, supporting the structural relationships proposed by the IBC model. Nonetheless, certain constructs, such as autonomy and controlled motivation were represented in a smaller subset of studies, which may slightly reduce the robustness of their associated simulated parameters.

	CM	AM	ATT	SN	PBC	INT	NFA
Mean	2.51	3.71	5.07	4.38	4.76	4.10	3.89
Standard Deviation	0.90	1.00	0.98	1.25	1.43	1.31	0.96
Correlations	CM	AM	AT	SN	PBC	IN	AU
CM	1						
AM	-0.25	1					
ATT	-0.25	0.61	1				
SN	-0.10	0.38	0.36	1			
PBC	-0.25	0.70	0.50	0.24	1		
INT	-0.25	0.56	0.48	0.33	0.48	1	
NFA	-0.25	0.45	0.50	0.45	0.40	0.45	1

Notes: CM: Controlled Motivation, AM: Autonomous Motivation, ATT: Attitude, SN: Subjective Norm, PBC: Perceived Behavioral Control, INT: Intention, NFA: Need for Autonomy. Source: Primary.

Table 1: Correlation Matrix of IBC constructs from Scoping Review

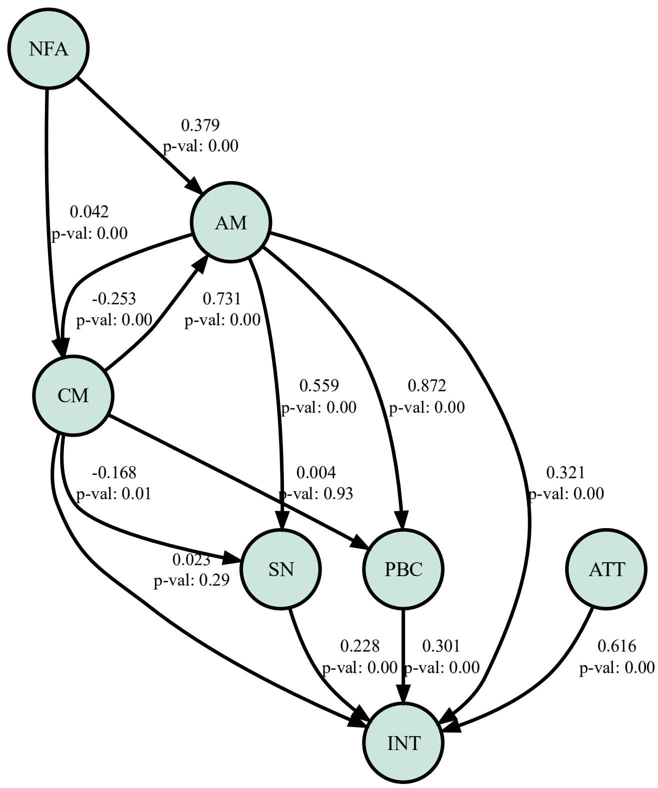
6.2 Simulated dataset

A total of N = 2,000 synthetic users were generated, each representing a virtual individual characterized by sociodemographic, psychological, and contextual attributes relevant to physical activity behavior (Table 2). Sociodemographic attributes were simulated to represent a plausible young adult Chilean population, encompassing age, gender, employment status, household composition, and baseline physical activity. This modeling process yielded the simulated population described in Table 2, which aligns with the behavioral profile targeted by the mHealth intervention.

Variable	Mean	Standard Deviation
Age (Years)	21.5	2.06
Gender (male = 1)	41.4%	
Employment		
• Full time	9.75%	
• Part time	31.20%	
• Unemployed	59.05%	
Household size (N)	3.2	1.23
Minors in household (N)	1.9	0.84
Physical Activity (Days per week)	2.39	0.84

Table 2: Simulated Sociodemographic attributes

The structural consistency of the dataset was validated through SEM analysis, fitting the adapted IBC model (Figure 4), reporting the partial correlations between constructs in the simulated data. The fitted model yielded a reasonable GFI (0.78) but a high RMSEA (0.53), well below desirable values, which is expected due to the simulated nature of the data. Contrasting with the findings summarized in Hagger & Chatzisarantis (2014), the estimated coefficients are somewhat higher than expected, but differences could arise from the population studied (children and adolescents versus university students and younger adults). However, the sign and significance of the estimated relationships confirmed that the simulated data preserved theoretical coherence and internal dynamics proposed by the IBC framework.



Notes: CM: Controlled Motivation, AM: Autonomous Motivation, ATT: Attitude, SN: Subjective Norm, PBC: Perceived Behavioral Control, INT: Intention, NFA: Need for Autonomy. Source: Primary.

Figure 4: SEM fitted on simulated data

The results from the predicted values from the CB learned policy on the simulated data are reported in Figure 5. We observe that the optimal (recommended) allocation differs significantly from starting random setup in the first cycle. Individuals in each difficulty level moved either to higher or lower difficulties, with most of them concentrating on difficulty 2 (moderate). Using the same function to predict behavior as used to generate the data on cycle 1, the optimal allocation yielded an average reward of 0.62, thus increasing 12 percent points relative to the initial allocation (50% adherence). Overall, these results suggest that, based on the simulated features from the IBC model, we can observe relevant sorting based on behavioral constructs measured in previous literature.

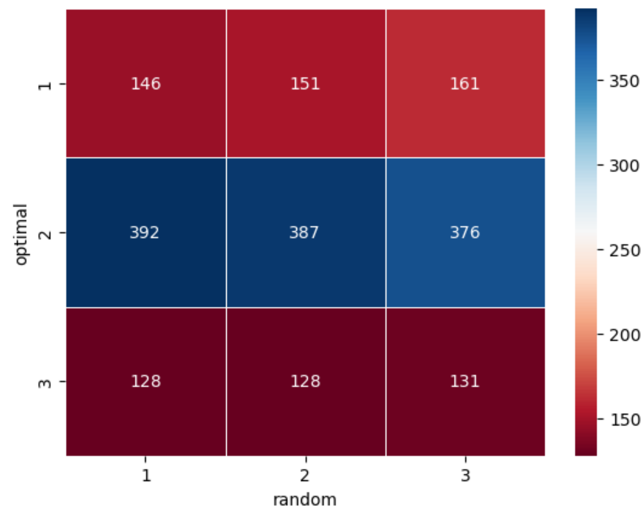


Figure 5: Transition matrix in difficulty assignment by cycle on simulated data

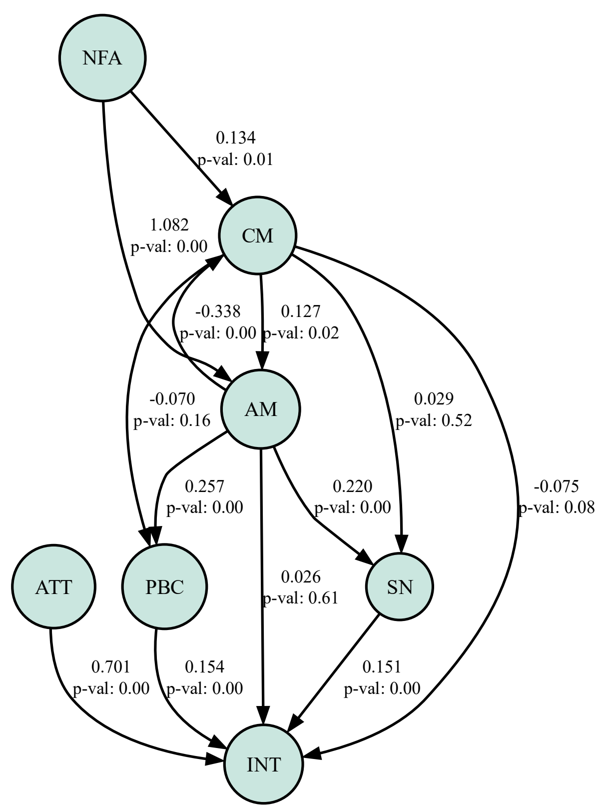
6.3 Pilot data

The dataset analyzed comprised a total of 558 students with ages ranging from 18 to 29 years old. From the initial placement questionnaire, we were able to obtain demographic characteristics (Table 3), to contrast with the simulated data. No substantial differences were found between the simulated values and the characteristics of the students participating in the pilot study, except in the employment variable, which showed a higher unemployment rate in the pilot sample than in the simulated population.

Variable	Mean	Standard Deviation
Age	23.9	6.52
Gender (male = 1)	44.3%	
Employment • Full time • Part time • Unemployed	 6,09% 22,50% 71,41%	
Household size (N)	3,41	1.52
Minors in household (N)	0.48	0.94
Physical Activity (Days per week)	2.51	1.50

Table 3: Pilot sociodemographic attributes

Using the IBC responses, we constructed a fully SEM model representing the pilot population, shown in Figure A2. Figure 6 contains a summarized version of the SEM model to contrast with the simulated data. The fitted model yielded a GFI of 0.85 and RMSEA 0.09, both borderline acceptable, considering the sample size. We observe how IBC constructs are interrelated in a similar fashion to the SEM fitted to the evidence-based simulated values. However, it is important to note that coefficients in real data are significantly smaller than the simulated values, except for the role of attitudes towards the activity. In particular we note that the role of autonomous motivation towards subjective norms and perceived behavioral control are significantly attenuated in relation to previously reported studies. While a single study is not enough to provide contrast, we can infer that university students in our sample have weakened pathways between autonomous motivation and intention towards the activity.



Notes: CM: Controlled Motivation, AM: Autonomous Motivation, ATT: Attitude, SN: Subjective Norm, PBC: Perceived Behavioral Control, INT: Intention, NFA: Need for Autonomy. Source: Primary.

Figure 6: Estimated SEM from Pilot data

Regarding adherence to the pilot implemented 252 users weren´t able or didn´t try to complete the first day of exercises, on the other hand the quantity of users that completed the subsequent quantity of days remains stable at an average of 51 users per day, meaning that only 50 users completed all 6 days, as seen in Figure 7. Again, we observed that the anticipated simulated adherence matched closely the pilot data results.

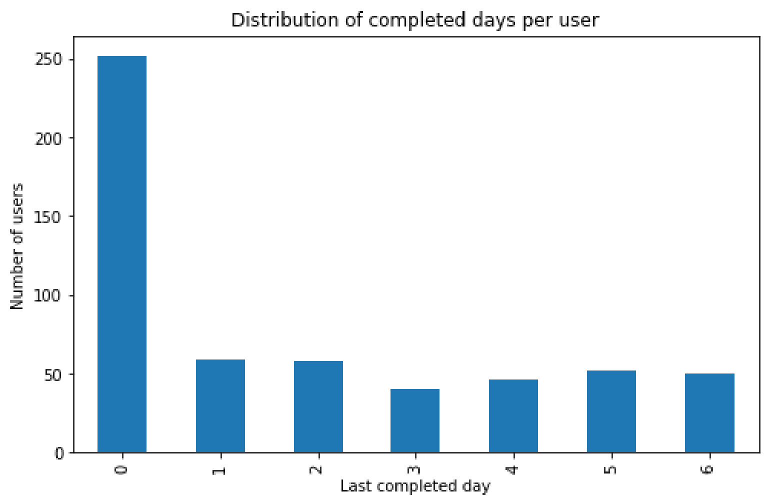


Figure 7. Completed days per user.

Finally, the results from the CB learning in the real data from the first cycle are shown in Figure 8. We observe that the allocation of individuals at each difficulty level was stable throughout both cycles of the pilot, with more stability at the moderate level. While there is less variation than in the simulated data, the patterns matched closely the re-allocation of individuals across levels. It is important to note that in the simulated example we only considered one day as cycle, while in the pilot, a cycle represents three consecutive days. We found significantly smaller success rates in the pilot data, however if we considered days completed, the results are somewhat similar (with smaller increments in average success between cycles).

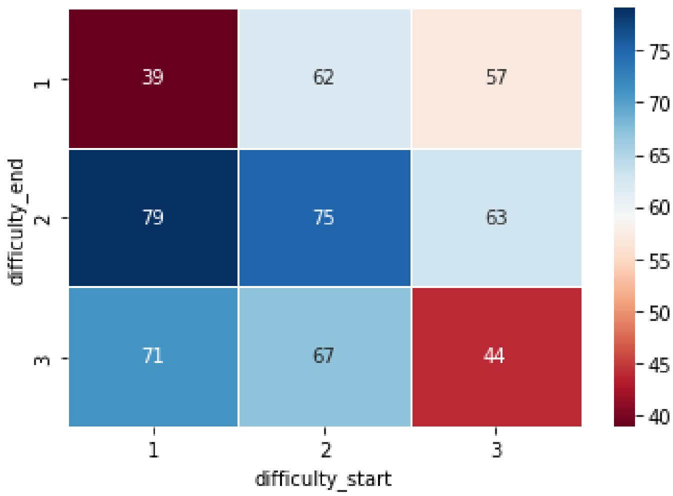


Figure 8: Transition Matrix

7. Discussion

This study explored the use of evidence-based synthetic data as a bridge between behavioral theory and algorithmic personalization in digital health. By creating synthetic users based on the average results of 18 empirical studies from a scoping review in Europe PMC database, we can contrast empirically informed simulated agents to the behavior of a real population of students participating in a mHealth physical activity intervention. We provide early evidence that simulations could be efficiently used to pre-train adaptive decision-making algorithms and help reduce the cold-start problem that usually limits personalization in the first interactions of mHealth applications.

The behavioral distributions obtained from the synthetic data were consistent with the conceptual structure of the IBC framework. The simulated users showed low pre-motivational awareness, moderate autonomous motivation, and high post-motivational determinants such as attitude, subjective norms, and perceived behavioral control. These patterns align with previous empirical evidence on physical activity adoption. For instance, Lemoyne et al. (2016) identified ATT and PBC as significant predictors of INT, highlighting their central role in shaping the intention to engage in physical activity.

Our results reveal that synthetic data generation based on behavioral theory offers a scalable and reproducible way to design and evaluate algorithms while protecting user privacy and avoiding early contact with clinical data. We also show how combining empirical calibration with reinforcement learning could eventually build a transparent methodological process that connects psychology with machine learning, making it potentially possible to assess different personalization hypotheses, such as how goal difficulty changes with self-efficacy. On the other hand, the similarity between simulated and real-world data suggests that synthetic data could also be used for continuous validation, helping to recalibrate algorithms as more real data become available.

Nevertheless, some limitations remain. The limited availability of data on IBC constructs may have influenced the accuracy of the simulation and the training of the CB model, primarily due to the underrepresentation of specific populations and regions. When the available evidence is scarce and predominantly derived from countries with similar socioeconomic or cultural profiles the resulting dataset may fail to capture the contextual, cultural, and environmental determinants that shape behavior in more diverse settings. This imbalance can lead to an overemphasis on certain internal or external factors, thereby reducing the ecological validity of the simulated users and constraining the generalizability of the model to populations with different characteristics. In our scoping review, for example, the constructs NFA and CM were represented by only two studies that provided correlation data with other constructs. Correspondingly, these constructs exhibited the largest discrepancies between the simulated SEM model and the pilot SEM model. To address this limitation, future implementations of this type of simulation should seek to incorporate the largest possible amount of data on IBC constructs and ensure that the populations represented in the source studies closely resemble the characteristics of the simulated population. Future work should include active learning mechanisms that allow the synthetic generator to adapt continuously based on real-world behavioral feedback. The application also presented some technical limitations that could be addressed in future iterations with additional development resources. For instance, implementing a native version of the web app for iOS and Android would not only enhance the user interface and overall experience but also enable the integration of built-in device sensors to collect richer data.

8. Conclusion

The present research set out to determine whether synthetic data informed by behavioral theory could effectively mitigate the CSP in the training of contextual bandit algorithms for personalized physical activity recommendations. The study developed and validated an integrative framework that combined empirical behavioral modeling, statistical simulation, and reinforcement learning. The results show that theory-driven synthetic data could potentially approximate the structure and behavioral logic of real user populations, providing a base for algorithmic pre-training prior to large-scale empirical deployment.

Overall, the research question whether theory-driven simulated data can solve the cold start problem in training contextual bandits for personalized physical activity recommendations can be answered affirmatively within the scope of this study. The findings confirm that behaviorally informed synthetic data could reduce the dependency on early empirical interactions, accelerate algorithmic convergence, and provide a potentially ethically safer, cost-efficient environment for preliminary model evaluation. The integration of psychological theory and machine learning not only enhances predictive performance but also strengthens interpretability and transparency key aspects for trust and accountability in digital health systems.

Nevertheless, the study also identified areas that warrant further development. The current simulator employed static distributions that did not account for temporal dynamics, contextual variability, or longitudinal feedback mechanisms that characterize real behavior change. Also, the application used to implement the pilot had many issues during the implementation which could have affected negatively sample size and adherence. On the other hand, for future studies we could implement better user interactions, mechanisms to improve adherence, also increasing the sample size of the pilot and extending the duration of the cycles or adding more cycles.

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Abbreviations

The following abbreviations are used in this manuscript:

CSP	Cold Start Problem
RL	Reinforcement Learning
IBC	Integrated Behavior Change
NCD	Non communicable diseases
mHealth	Mobile Health
CB	Contextual Bandits
TPB	Theory of Planned Behavior
SDT	Self Determination Theory
UCB	Upper Confidence Bound
AM	Autonomous Motivation
ATT	Attitude
SN	Subjective Norm
PBC	Perceived Behavioral Control
INT	Intention
NFA	Need for Autonomy
CM	Controlled Motivation
BREQ-2/3	Behavioral Regulation in Exercise Questionnaire
GSLTPAQ	Godin-Shepard Leisure-Time Physical Activity Questionnaire
ADP	Action Dependant Feature
SEM	Structural Equation Model

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Supplemental Annex

Table A1. Literature Review Article Summary

Title	Author , year	Country	DOI
From Physical Activity Intention to Behavior: The Moderation Role of Mental Toughness Among College Students and Wage Earners	(Cao et al., 2021)	China	10.3389/fpsyg.2021.584760
The role of companionship, esteem, and informational support in explaining physical activity among young women in an online social network intervention	(D. N. Cavallo et al., 2014)		10.1007/s10865-013-9534-5
Extended Theory of Planned Behavior on Eating and Physical Activity	(Cheng et al., 2019)	Hong Kong	10.5993/ajhb.43.3.11
A daily process analysis of intentions and physical activity in college students	(Conroy et al., 2013)	United States of America	10.1123/jsep.35.5.493
Improving Physical Activity Levels and Psychological Variables on University Students in the Contemplation Stage	(Corella et al., 2019)	Spain	10.3390/ijerph16224368
Predictors of Self-Determined Module Choice in a Web-Based Computer-Tailored Diet and Physical Activity Intervention: Secondary Analysis of Data From a Randomized Controlled Trial	(Coumans et al., 2020)	Holland	10.2196/15024
Understanding Physical Activity and Exercise Behavior in China University Students: An Application of Theories of the Flow and Planned Behavior	(Feng et al., 2022)	China	10.1155/2022/7469508
An Integrated Behavior Change Model for Physical Activity	(Hagger & Chatzisarantis, 2014)	N/A	10.1249/JES.0000000000000008
Analyzing Exercise Behaviors during the College Years: Results from Latent Growth Curve Analysis	(Lemoyne et al., 2016)	Canada	10.1371/journal.pone.0154377

Physical activity levels and self-determined motivation among future healthcare professionals: Utility of the Behavioral Regulation in Exercise Questionnaire (BREQ-2)	(Mahony et al., 2019)	Ireland	10.1080/09593985.2018.1457112
Use of Wearable Technology and Social Media to Improve Physical Activity and Dietary Behaviors among College Students: A 12-Week Randomized Pilot Study	(Pope et al., 2019)	United States of America	10.3390/ijerph16193579
Self-determined Engagement in Physical Activity and Sedentary Behaviors of US College Students	(Quartiroli & Maeda, 2014)	United States of America	10.70252/svgj1383
Do sedentary motives adversely affect physical activity? Adding cross-behavioural cognitions to the theory of planned behaviour	(Rhodes & Blanchard, 2008)	Canada	10.1080/08870440701421578
Motivation Regarding Physical Exercise among Health Science University Students	(Sánchez-Herrera et al., 2022)	Spain	10.3390/ijerph19116524
Motivation and Physical Activity: Differences Between High School and University Students in Spain	(Sevil et al., 2018)	Spain	10.1177/0031512518788743
The Role of Triggers in Physical Activity among College Students: An Extended Model of the Theory of Planned Behavior	(Wang & Kang, 2024)	China	10.3390/bs14040328
The Value-Added Contribution of Exercise Commitment to College Students' Exercise Behavior: Application of Extended Model of Theory of Planned Behavior	(Zhang et al., 2022)	China	10.3389/fpsyg.2022.869997
Physical activity motivations and psychological well-being among university students: a canonical correlation analysis	(Zhong, 2024)	China	10.3389/fpubh.2024.1442632

Table A2. Behavioral questionnaire for IBC constructs

N°	IBC Construct	Question	Scale
	CM	Please indicate below whether or not the statements below are true for you	
Q17	CM	I work out because other people say I should.	1 to 5
Q19	CM	I work out because others will be disappointed if I don’t.	1 to 5
Q24	CM	I feel under pressure from my friends/peers/partner to work out.	1 to 5
	AM	Please indicate below whether or not the statements below are true for you	
Q26	AM	It is pleasurable to work out.	1 to 5
Q27	AM	It is important to me to work out.	1 to 5
Q28	AM	I enjoy working out	1 to 5
	ATT	For me, working out during the next four weeks would be…	
Q33	ATT	Unimportant-Important	1 to 7
Q34	ATT	Not worthwhile-Worthwhile	1 to 7
Q35	ATT	Harmful-Beneficial	1 to 7
	SN	Do you agree with the following statements?	
Q39	SN	Most people who are important to me would want me to work out during the next four weeks.	1 to 7
Q40	SN	Most people I know would approve of me working out during the next four weeks.	1 to 7
Q42	SN	Most people who are relevant to me would approve of me working out during the next four weeks	1 to 7
	PBC	Do you agree with the following statements?	
Q44	PBC	How much personal control do you have over working out over the next four weeks?	1 to 7
Q45	PBC	It is mostly up to me whether or not I work out during the next four weeks	1 to 7
Q46	PBC	If I wanted to, I could work out during the next four weeks.	1 to 7
Q47	PBC	Working out during the next four weeks is up to me.	1 to 7
	INT	Do you agree with the following statements?	
Q49	INT	I intend to work out during the next four weeks.	1 to 7
Q50	INT	I plan to work out during the next four weeks.	1 to 7
Q51	INT	I will try to work out during the next four weeks.	1 to 7
Q56	NFA	If I had to change my behaviour to get healthier, I would motivate myself	1 to 7
Q57	NFA	If I had to change my behaviour to get healthier, I would ask family and friends to motivate me	1 to 7
Q58	NFA	If I had to change my behaviour to get healthier, I would ask an expert to motivate me	1 to 7

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Figure A1. Complete SEM model for pilot data