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The iterative development and refinement of health psychology theories through formal, dynamical systems modelling: a scoping review and initial expert-derived 'best practice' recommendations

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ABSTRACT

This scoping review aimed to synthesise methodological steps taken by researchers in the development of formal, dynamical systems models of health psychology theories. We searched MEDLINE, PsycINFO, the ACM Digital Library and IEEE Xplore in July 2023. We included studies of any design providing that they reported on the development or refinement of a formal, dynamical systems model unfolding at the within-person level, with no restrictions on population or setting. A narrative synthesis with frequency analyses was conducted. A total of 17 modelling projects reported across 29 studies were included. Formal modelling efforts have largely been concentrated to a small number of interdisciplinary teams in the United States (79.3%). The models aimed to better understand dynamic processes (69.0%) or inform the development of adaptive interventions (31.0%). Models typically aimed to formalise the Social Cognitive Theory (31.0%) or the Self-Regulation Theory (17.2%) and varied in complexity (range: 3-30 model components). Only 3.4% of studies reported involving stakeholders in the modelling process and 10.3% drew on Open Science practices. We conclude by proposing an initial set of expert-derived 'best practice' recommendations. Formal, dynamical systems modelling is poised to help health psychologists develop and refine theories, ultimately leading to more potent interventions.

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Introduction

Modifiable health behaviours including tobacco smoking, alcohol consumption, low physical activity, unhealthy dietary behaviour, unsafe sexual health behaviour, and poor medication adherence are leading preventable causes of premature morbidity and mortality (de Ridder et al., 2017; de Wit et al., 2022; Kuntsche et al., 2017; Rhodes et al., 2017; Stewart et al., 2022; West, 2017). Understanding how to predict, explain, and influence health behaviours is one of the most pressing issues facing health psychologists. In this service, our field has been occupied with the development and

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refinement of theories – broadly defined here as 'a systematic way of understanding events or situations. It is a set of concepts, definitions, and propositions that explain or predict these events or situations by illustrating the relationships between variables' (Glanz & Rimer, 2005) – with a view to devising effective interventions which can engender improved health and wellbeing for all. However, progress is hindered by the 'reproducibility crisis' in general (Munafò et al., 2017; Nosek et al., 2018) and the 'theory crisis' in particular – i.e., our available health psychology theories exist as underspecified box-and-arrow diagrams and imprecise natural language descriptions of the interrelationships between constructs (Eronen & Bringmann, 2021; Oberauer & Lewandowsky, 2019). More specifically, our theories are 'weak' – i.e., they do not strongly imply testable hypotheses, but researchers must first add a substantial number of auxiliary assumptions about the study design and measurement of social reality constructs (see [Peters & Crutzen, 2024] for a detailed discussion about the 'measurement crisis'). This makes it impossible to systematically develop, test, and refine our theories, which in turn stifles progress towards our central goal: improving understanding of health behaviours and devising effective interventions.

Thus far, health psychology theories such as the Social Cognitive Theory and the Self-Regulation Theory have been developed based on (and used to inform) studies that have been characterised as falling within a 'low-resolution measurement paradigm' (Chevance, Perski et al., 2021; Riley et al., 2011). This is illustrated by the high volume of health psychology studies which have adopted cross-sectional or longitudinal (non-intensive) survey designs and pre- and post-intervention study designs to examine between-person associations or estimate the average (between-group) treatment effect (Chevance, Perski et al., 2021; Spruijt-Metz et al., 2015). Recent technological and methodological advances, however, including the widespread uptake and use of smartphones and wearable devices, have enabled researchers and practitioners to capture health behaviours at high sampling frequencies in people's daily lives and at the within-person level. For example, a recent systematic review identified >600 studies that used Ecological Momentary Assessments (EMAs) to study how health behaviours unfold within and between individuals in real-life contexts (Perski et al., 2022). Compared with previous empirical observations that were made under the 'low-resolution measurement paradigm' (e.g., measurements taken at baseline and at a 3- and 6-month follow-up), observations facilitated by these technological and methodological advances have also enabled (and challenged) researchers to consider that many health behaviours display characteristics of dynamical systems (Baretta et al., 2023; Chevance, Perski et al., 2021; Chevance, Baretta et al., 2021; Heino et al., 2021). A dynamical system is any system (e.g., a population, an individual) which changes over time in response to different inputs (e.g., motivation, weather). Dynamical systems modelling provides a mathematical framework for understanding and predicting dynamical systems by formulating a series of rules or equations which describe how the system changes over time. Importantly, the state of the system at any time point is determined by its initial state and its evolution over time based on the rules (Sayama, 2015). Recent studies have shown that health behaviours such as physical activity, cigarette smoking and alcohol consumption fluctuate irregularly and non-linearly over time (e.g., from day to day, or hour to hour) in response to time-varying internal and external factors (Businelle et al., 2016; Chevance, Baretta et al., 2021; Chevance, Perski et al., 2021; Hekler et al., 2019; Perski et al., 2019). In addition, research shows that these fluctuations can be idiosyncratic (i.e., they differ from person to person), which may make group-to-individual generalisability unreasonable to assume (Fisher et al., 2018). Studies have also shown that feedback loops occur within individuals over time, with recursive relationships between behaviours (e.g., physical activity, sleep) and/or psychological constructs (e.g., self-efficacy, positive affect, negative affect) observed in studies that fall within a 'high-resolution measurement paradigm' (Lydon-Staley et al., 2021; McGowan et al., 2023). Importantly, these recent observations have highlighted the inherent 'complexity' and 'system-ness' of many health behaviours (Heino et al., 2021), which cannot be adequately represented using formalisms that have traditionally been used to develop and refine health psychology theories (e.g., applying mediation/moderation techniques to cross-sectional data) (Hofmann et al., 2020). At the same time, health psychologists have begun to recognise that, to make progress on the most pressing issues of our times (e.g.,

addiction, obesity, mental health, and climate change), we must become better able to theorise about and influence dynamical systems (Chevance et al., 2023; Gomersall, 2018; Heino et al., 2021).

A strong candidate approach for counteracting the theory crisis is the use of 'formal modelling' – i.e., the translation of a theory's structure into a mathematical framework – e.g., a series of mathematical equations or logical statements (Borsboom et al., 2021; Chevance, Perski et al., 2021; Farrell & Lewandowsky, 2010; Fried, 2020; Guest & Martin, 2021; Haslbeck et al., 2021; Robinaugh et al., 2021; Smaldino, 2017; van Rooij & Blokpoel, 2020). It should be noted that both explanatory theories and their formalised counterparts are intended to be interpreted causally (i.e., the theory explains how the phenomenon of interest arises). As such, the development of a formal model which acts as the 'empirical interface' of a given theory allows a variety of empirical studies to be conducted. In turn, interpreted observations generated from these empirical studies (e.g., data collected via EMAs or wearable sensors, qualitative interviews with people with lived experience) have clearly expected effects of strengthening, weakening, or changing the theory (Guest, 2023; Guest & Martin, 2021). It is important to highlight how formal modelling differs from related computational approaches, such as machine learning. Machine learning is largely a data-driven approach, where functions (i.e., input-output mappings) are learnt directly from the data. Partly due to their flexible structure, machine learning algorithms can capture complex relationships, but this comes at the cost of limited interpretability (Henninger et al., 2023). Formal modelling, on the other hand, relies largely (but not solely) on abduction – i.e., reasoning and inference to the best explanation (Borsboom et al., 2021; Haig, 2005). As such, formal models are less flexible than machine learning algorithms, but more precise and verifiable. As mentioned above, learning from data is an important part of the formal modelling process, but it is only one piece of the puzzle. The use of formal modelling was pioneered within the health psychology field by translating the Theory of Planned Behaviour (Navarro-Barrientos et al., 2011) and subsequently the Social Cognitive Theory (Martín et al., 2018; Riley et al., 2016) into a series of differential equations. This was followed by a sequence of 'system identification' experimental studies to test and iteratively refine the formal model at the within-person level (Park et al., 2023; Phatak et al., 2018). See Box 1 for a practical example of the translation of the Social Cognitive Theory into a formal, dynamical systems model. The addition of a dynamical systems lens to the formal modelling process (i.e., not simply the use of any mathematical or logical formalism, but specifically the use of formalisms that can accommodate non-linear, recursive causal relationships, such as time series analysis, Bayesian dynamic models, state-space models, etc) has the potential to narrow the gap between emerging empirical evidence generated under a 'high-resolution measurement paradigm' and our current health psychology theories, which were mostly developed and tested under a 'low-resolution measurement paradigm' (Chevance, Perski et al., 2021).

Box 1. Example of how the Social Cognitive Theory was translated into a formal, dynamical systems model.

In a series of publications, an interdisciplinary research team set out to formalise Bandura's Social Cognitive Theory (Martín et al., 2018; Riley et al., 2016), which proposes that human behaviour arises due to the interaction of attributes of the person (e.g., self-efficacy, outcome expectancies), their behaviour, and their environment (e.g., others' behaviours) – referred to as 'reciprocal determinism' or a 'triadic causation model'. As such, Bandura implicitly proposed that human behaviour can be represented as a dynamical system with feedback loops.

The first step of the formalisation process involved clearly specifying the constructs of interest (e.g., self-efficacy, outcome expectancies, behavioural outcomes, self-management skills) and their interrelationships. For example, it was proposed that self-management skills influence self-efficacy and outcome expectancies.

Next, the expected interrelationships were translated into a series of mathematical equations. For example, the change in self-management skills (η_1) with respect to time was represented as a function of itself at time *t*, skills training at time *t*, behaviour at time *t* and disturbances at time *t*. In turn, the change in self-management skills was represented as influencing other theoretical constructs (e.g., self-efficacy), according to the interrelationships specified in the first step.

In the final step, the system dynamics were simulated through selecting plausible parameter values (i.e., numeric weights/constants) for the different inputs. Next, the parameter values were estimated from real-world data, retaining the pre-specified model structure, and allowing the parameters to take different plausible values. Visual inspection of the time series plots of the simulated and the real-world output data, in addition to calculating the percentage fit between the time series, led to refinements of the model structure.

The researchers concluded that the formalisation process, simulations, and fitting the dynamical systems model to real-world data was useful for specifying many implicit assumptions of the Social Cognitive Theory and testing different scenarios that were considered more/less plausible. As a consequence, going through the formal modelling cycle served as a direct test of the Social Cognitive Theory and led to further theory refinements.

In addition to having the potential to bridge the gap between emerging empirical observations and currently under-specified and static health psychology theories, there are additional reasons why formal, dynamical systems modelling constitutes a useful addition to the health psychologist's toolbox. First, it can help enable greater consilience between seemingly disparate phenomena that operate across different systems levels and timescales (e.g., micro-scale brain 'computations' involved in decision-making or learning, macro-scale interactions between agents in a neighbourhood or city). 'Scale bridging methodologies', which are commonly used as part of multiscale modelling efforts in engineering, physics, chemistry, biology, and public health can enable theorising about health behaviours at different spatiotemporal scales (Hoekstra et al., 2014). For example, despite implicit theorising that some psychological processes are fast- and others are slow-evolving processes (e.g., affect and social identity, respectively), to our knowledge, few theories and empirical studies have examined the different temporal dynamics with formal explication on exactly how to operationalise and distinguish 'fast' and 'slow' processes. In a formal, dynamical systems model, however, researchers can explicitly incorporate the expected dynamics beyond natural language descriptions. This can also help with the development of standards for the sampling frequency of psychological constructs, instead of perpetuating unprincipled or strictly pragmatic sampling practices, such as sampling rates selected based on past convention (e.g., measurements taken at baseline and at 3- and 6-month follow-ups).

Second, a dynamical systems lens allows researchers to incorporate historically important and fundamental psychological processes such as habituation or learning into our theories, which can only be meaningfully conceptualised and modelled over time and within individuals. Third, the formalisation of theories facilitates in silico analyses (i.e., computer simulations) of the dynamics of the focal system under varying conditions (e.g., following the introduction of an intervention or policy), thus allowing researchers to explore issues of interest that would be difficult or impossible for ethical reasons or due to a lack of resources to measure in a study. Such simulations can support theory refinement and, in turn, the generation of more precise hypotheses to be empirically tested pending increased resource or improved measurement instruments, as evidenced within refined 'system identification' experiments (Park et al., 2023; Phatak et al., 2018). Fourth, formal, dynamical systems modelling is poised to accelerate the development of adaptive interventions, including but not limited to 'just-in-time adaptive interventions' (JITAIs), which aim to provide the right type of support to individuals at the right time (Hardeman et al., 2019; Nahum-Shani et al., 2016; Perski et al., 2021). The iterative process of formal, dynamical systems modelling allows for a progressively better understanding of within-person dynamics, which is required for robust control to achieve desired health outcomes (Collins et al., 2004; Rivera et al., 2007). To date, however, few JITAIs have been underpinned by formal modelling efforts (Perski et al., 2021).

Arguably, formal, dynamical systems modelling as a method for iteratively developing and refining health psychology theories is necessary for researchers and decision-makers to tackle the biggest challenges facing our societies today. Although several scientific disciplines (e.g., ecology, biology, engineering, physics, neuroscience, psychiatry) have engaged in formal modelling extensively for decades (Chen et al., 2015; Huys et al., 2016; Montague et al., 2012; Nassar & Frank, 2016; Stephan & Mathys, 2014; Wilson & Collins, 2019), its use in health psychology remains relatively rare. With a view to making theory development and refinement through formal, dynamical systems modelling more accessible to health psychologists, we therefore aimed to conduct a scoping review to summarise the extent and nature of activities relating to the formal modelling of health psychology theories pertaining to health behaviours that unfold at the within-person level. We aimed to synthesise methodological steps, reflect on these from the perspective of an interdisciplinary expert

review team, and provide a set of initial expert-derived 'best practice' recommendations for health researchers who intend to use formal, dynamical systems modelling in their future work. To ensure the review remained sufficiently focused and to avoid overlap with available reviews of agent-based models in public health (Boyd et al., 2022; Nianogo & Arah, 2015; Tracy et al., 2018; Yang, 2019), we focused here on within-person processes (as opposed to agent-agent interactions, as in agent-based models), which also aligns with the proposition that useful health psychology theories should apply to individuals (Johnston & Johnston, 2013). It should, however, be noted that formal, dynamical systems models can account for between-person processes or variables in different ways. For example, social interactions including social influence could be explicitly modelled (which is typically the case in agent-based models), with the agents having different between-person characteristics (e.g., age, gender, socioeconomic position). Traditional between-person variables could also be implicitly incorporated in a within-person dynamical systems model through varying the starting conditions or parameter values. For example, if a theory proposes that individuals have different probabilities of stress exposure or reactivity depending on their age, gender, or socioeconomic position, this could be incorporated into a formal, dynamical systems model's structure.

Specifically, this scoping review aimed to address the following research questions (refined following the pre-registration of the review protocol, as discussed in the 'Data items and data collection process' subsection of the 'Methods'):

- (1) In which areas of health behaviour research has formal, dynamical systems modelling been used to develop, test and/or refine theory?
 - a. What team expertise was considered useful?
 - b. What were the researchers' modelling objectives?
- (2) What methodological steps have researchers taken as part of the formal modelling process?
 - a. Have stakeholders been involved in the formal modelling process and if so, how?
 - b. What sources of knowledge have been used to identify the model components and structure?
 - c. Has iteration been used as part of the modelling process and if so, how?
 - d. Have internal (e.g., use of simulation) and/or external (e.g., fit to real-world data) consistency checks been carried out?
- (3) How clear and comprehensive is the model reporting?
 - a. Are descriptions of the model components and structure provided?
 - b. Have justifications for the model time steps (i.e., points in time at which the model makes calculations or predictions) and run length (i.e., the total length of time the model is set to run to observe its behaviour) been provided?
 - c. Have researchers reported what mathematical frameworks/formalisms and software were used?
 - d. Is pseudo-code and/or code openly available?
 - e. What did researchers report having learnt from their modelling efforts?

Methods

Study design

This was a scoping review, which followed the methodological guidelines developed by Arksey and O'Malley (2005), extended by Levac and colleagues (Levac et al., 2010) and Peters and colleagues (Peters et al., 2015). We opted for a scoping, rather than a systematic, review as the use of formal, dynamical systems modelling in health behaviour research is still in its infancy. Therefore, a focus on methods and applications across a diverse range of studies was judged to be most useful. As there is no agreed-upon method for evaluating the quality of or potential risk of bias within formal modelling studies in health behaviour research, standard assessment tools used for such

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purposes in systematic reviews were not considered appropriate. The scoping review protocol was pre-registered on the Open Science Framework (https://osf.io/7htkd); however, this was necessarily minimalistic and required several refinements during the review process (see details below). The PRISMA extension for scoping reviews (PRISMA-ScR) was used in the design of the review protocol and the checklist was used in the reporting of the review results (Tricco et al., 2018) (see the Supplementary Materials 1).

Eligibility criteria

We included studies of any design (e.g., conceptual, empirical) providing that they reported on the development, refinement and/or testing of a formal, dynamical systems model of a health behaviour or a health behaviour theory unfolding at the within-person level. We defined a formal, dynamical systems model as any explanatory theory or framework which proposes that health behaviour is the output of a dynamical system with recursive relationships, providing that the explanatory theory or framework was represented using a mathematical framework (e.g., difference equations, differential equations) and where the development process relied at least in part on abduction (rather than solely on induction). In addition, the formal, dynamical systems model needed to operate at the within-person level, as several published reviews have focused on the formal modeling of agent-agent interactions and between-person processes (Boyd et al., 2022; Nianogo & Arah, 2015; Tracy et al., 2018; Yang, 2019). There were no restrictions on age group (e.g., child, adolescent, adult, older adult) or setting (e.g., country, city). Health behaviours were defined here as 'any activity undertaken for the purpose of preventing or detecting disease or for improving health and wellbeing' (Conner & Norman, 2015).

Information sources and search strategy

We searched MEDLINE, PsycINFO, the ACM Digital Library and IEEE Xplore in July 2023. Terms were searched for in titles and abstracts as free text or index terms (e.g., Medical Subject Headings), as appropriate. Three groups of terms were combined: the first group included terms related to health behaviours (e.g., 'tobacco smoking', 'alcohol consumption', 'substance use', 'physical activity', 'sedentary behaviour', 'dietary behaviour', 'medication adherence', 'sexual health behaviour', 'sleep', 'hand hygiene', 'cancer screening'). The second included terms related to formal, dynamical systems modelling (e.g., 'formal model', 'mathematical model', 'computational model', 'dynamical systems model', 'drift diffusion model', 'Markov model', 'difference equation', 'differential equation', 'control engineering', 'time series', 'state-space model'). The third included terms related to within-person processes (e.g., 'within-person', 'individual', 'idiographic'). Due to observed differences in retrieval qualities between academic search systems (e.g., use of Boolean operators, use of truncations and wildcards, use of '') (Gusenbauer & Haddaway, 2020), the final search string for each database was tweaked to fit its architecture. The search was restricted to human studies available in English that were published in peer-reviewed journals (see the Supplementary Materials 2).

In addition to the electronic searches, we scanned the reference lists in the included studies (backwards reference chaining) and ran a search for studies that cited the included studies (forwards reference chaining). Expertise within the review team was used to identify additional studies.

Study selection

Identified records were merged and duplicate records were removed. OP screened the titles and abstracts against the pre-specified eligibility criteria, with a random 20% of titles and abstracts independently screened by AC. Any discrepancies, including the need to further refine the eligibility criteria definitions (e.g., the definition of a dynamical system, the definition of a formal model), were resolved through discussion and through involving GC if needed. OP subsequently went back over all the

screening decisions, applying the refined eligibility criteria. Next, full texts were independently screened, following the same procedure as for the title and abstract screening. A primary reason for exclusion was recorded at the full text stage (Moher et al., 2009). Inter-rater reliability was not assessed.

Data items and data collection process

A data extraction form was iteratively developed in Microsoft Excel through discussion among the review team about methodological steps that we, as experts in formal, dynamical systems modelling, believe are important. Some data items had been specified in the pre-registration of the review protocol to align with the research questions (e.g., whether and if so, how, stakeholders were involved; whether empirical data were leveraged; whether any model testing/validation techniques and sensitivity checks were deployed). However, after piloting the data extraction form on the first 10% of included studies and following several rounds of discussion among the review team, a few amendments were made to the research questions and the corresponding data items (including their definitions and extractor instructions). We thus extracted information on: (i) the study characteristics (i.e., authors; year of publication; country; team expertise and the authors' reflections on what expertise was considered useful; the health behaviour of interest; the modelling purpose/objective; and the time required to complete the modelling effort), (ii) the modelling methods (i.e., whether and if so, how, stakeholders were involved (defined here broadly as individuals with an interest in, but not direct responsibility for, the modelling efforts - e.g., 'external' researchers from different scientific disciplines, people with lived experience, health practitioners, industry professionals, leaders of community organisations, policy makers, and so on); what sources of knowledge were used to identify the model components and structure; internal consistency checks, including the use of simulation, descriptions of the simulated participant characteristics, whether a simulation benchmark(s) was defined, and sensitivity checks on the parameter values or other assumptions; external consistency checks, including whether the model was fit to real-world data and the calculation of goodness-of-fit statistics, descriptions of the participant characteristics, and any model comparison(s); and the use of iterative modelling practices), and (iii) the clarity and comprehensiveness of the model reporting (i.e., the mathematical framework/formalism and software used; the model time steps and run length and justifications for these; whether a schematic of the model components and structure was provided; a summary of the model components; and the modelling outcomes). See the Supplementary Materials 2 for the final data item definitions and the extractor instructions used.

OP extracted the data. In the pre-registration, we had specified that data from a random 20% of the included studies would be independently extracted. However, given the complexity of many of the included modelling papers, an amendment was made to independently double check the extracted data from 100% of the included studies. The double checking was performed by AC, JA, and GC using the final list of data item definitions and the extractor instructions. Any discrepancies were resolved through discussion. A few lengthy data items benefitted from being further reduced prior to the frequency analysis (e.g., the modelling purpose/objective, the modelling outcomes). These were inductively coded by OP and amended following discussion with GC (see the Supplementary Materials 3).

Quality appraisal

Consistent with methodological guidance on scoping reviews, we did not appraise the quality or risk of bias of the included studies (Arksey & O'Malley, 2005; Levac et al., 2010; Peters et al., 2015).

Data synthesis

A narrative synthesis with frequency analyses was conducted. Due to the relatively small number of included studies, the findings were arranged according to the research questions (as opposed to, for

example, the health behaviour or theory of interest). Through reflection on the review findings and discussion within the review team, we subsequently proposed an initial set of expert-derived 'best practice' recommendations for health researchers interested in applying formal, dynamical systems modelling in their future work. These initial recommendations were not intended to be comprehensive (e.g., through synthesising recommendations across the interdisciplinary formal modelling literature); we reflected instead on the practices observed in the reviewed studies and what we, as an interdisciplinary team of experts with knowledge and experiences of formal, dynamical systems modelling, would encourage researchers to consider going forwards.

Results

A total of 1,872 records were identified for the title and abstract screening, with 70 full texts screened. An additional 14 full texts were identified through reference chaining and expertise within the review team. Of these, 17 modelling projects reported across 29 studies were included (see Figure 1; see the Supplementary Materials 3 for a mapping between the projects and studies). Given important nuances across the studies reporting on activities pertaining to the same modelling project, the denominator in the narrative synthesis was set to the study rather than the project level.

Study characteristics

Most studies were conducted in the United States (23/29; 79.3%) and were published between 1984 and 2022 (see Table 1). The modelling efforts were focused on physical activity (10/29; 34.5%), cigarette smoking (4/29; 13.8%), any (i.e., a non-specified) health behaviour (3/29; 10.3%), multiple health behaviours (i.e., the simultaneous study of physical activity and eating behaviour, 3/29; 10.3%), general substance use (3/29; 10.3%), alcohol consumption (2/29; 6.9%), cocaine use (1/29; 3.4%), or eating behaviour (1/29; 3.4%).

The modelling teams included researchers and practitioners from mathematics/engineering departments (20/29; 69.0%), psychology/behavioural science/cognitive science departments (14/29; 48.3%), public health/epidemiology departments (13/29; 44.8%), computer science departments (8/29; 27.6%), medicine/psychiatry departments (4/29; 13.8%), and neuroscience departments (3/29; 10.3%). Most studies (27/29; 93.1%) did not provide a reflection as to what expertise was considered useful in the modelling process. Two studies mentioned that an interdisciplinary approach is needed



Figure 1. Preferred Reporting Items for Systematic Reviews and Meta-Analyses (PRISMA) flow diagram of included studies.

| Authors (year) | Country | Health behaviour (s) | Team expertise | Modelling purpose/ objective | Time required for modelling |
|--------------------------------|---------------|--|---|---|-----------------------------------|
| Banks et al. (2014) | United States | Alcohol consumption | Psychology, mathematics, epidemiology, and engineering; a reflection on what expertise was considered useful is not provided. | To improve understanding of the behavioural mechanisms underpinning drinking behaviour. | Not reported. |
| Banks et al. (2017) | United States | Alcohol consumption | Data science and neuroscience; a reflection on what expertise was considered useful is not provided. | To help understand mechanisms of behaviour change in problem drinkers. | Not reported. |
| Baretta et al. (2019) | Italy | Physical activity | Psychology and applied mathematics; a reflection on what expertise was considered useful is not provided | To develop a computational model of behaviour change, which can be used to propose adaptive physical activity goals | Not reported. |
| Berardi et al. (2018) | United States | Any health behaviour | Psychology, mathematics, epidemiology, and engineering; a reflection on what expertise was considered useful is not provided | To develop a computational model of behaviour shaping, with a view to leveraging the model in future just-in-time adaptive interventions | Not reported. |
| Bobashev et al. (2017) | United States | Cigarette smoking | Data science and neuroscience; a reflection on what expertise was considered useful is not provided. | To develop a multi-scale computational model that simulates realistic daily smoking patterns and links to visualisations of brain areas that are activated during binge/ intoxication, withdrawal, and craving. | Not reported. |
| Caselles et al. (2010) | Spain | Cocaine use | Psychology and applied mathematics; the authors mention that an interdisciplinary approach is needed when modelling complex systems but do not further elaborate on this | To present a dynamic model of a stimulant drug addiction (cocaine) that integrates personality, the acute effect of the drug, and addiction. | Not reported. |
| Dong et al. (2012) | United States | Eating behaviour and physical activity | Engineering, mathematics, and public health; a reflection on what expertise was considered useful is not provided. | To present a dynamical systems model that describes how a behavioural intervention can influence weight gain during pregnancy, which can be used to underpin future adaptive interventions | Not reported. |
| El Mistiri et al. (2022) | United States | Physical activity | Engineering and public health; a reflection on what expertise was considered useful is not provided. | To improve understanding of multi-timescale behavioural dynamics (i.e., within-day and day- to-day) within the context of an adaptive digital intervention for physical activity | Not reported. |
| Ghosh (2015) | United States | Any health behaviour (cigarette smoking is used as case study) | Computer science; a reflection on what expertise was considered useful is not provided. | To develop a formal model of persuasive actions for behaviour change, within the context of mobile and wearable devices. | Not reported. |

Table 1. Characteristics of the included studies.

Table 1. Continued.

| Authors (year) | Country | Health behaviour (s) | Team expertise | Modelling purpose/ objective | Time required for modelling |
|-----------------------------|--------------------------|-------------------------|---|---|-----------------------------------|
| Giraldo et al. (2017) | United States | Alcohol consumption | Engineering; a reflection on what expertise was considered useful is not provided. | To improve understanding of the dynamic interplay between the environment, the interactions between individuals, and personal motivations and characteristics that affect unhealthy patterns of consumption during drinking events. | Not reported. |
| Giraldo et al. (2017) | United States | Alcohol consumption | Engineering; a reflection on what expertise was considered useful is not provided. | To propose a model that explains the 'physics' of an individual's blood alcohol content (BAC) during a drinking event (i.e., how the output of the decision-making process translates into BAC variations and how BAC variations in turn affect decision-making). | Not reported. |
| Grasman et al. (2016) | The Netherlands | Substance use | Mathematics and psychology; a reflection on what expertise was considered useful is not provided. | To explore the applicability of a dynamical systems approach in the analysis of addictive behaviours and the development of addiction. | Not reported. |
| Guastello (1984) | United States | Substance use | Mathematics and psychology; a reflection on what expertise was considered useful is not provided. | To explore whether the class of theories referred to as 'opponent process models' that underpin addictive behaviours can be considered examples of cusp and butterfly catastrophes. | Not reported. |
| Klein et al. (2013) | The Netherlands | Any health behaviour | Computer science and cognitive science; a reflection on what expertise was considered useful is not provided. | To understand and detect the causes of unhealthy behaviour to devise tailored interventions via an intelligent coaching system | Not reported. |
| Levy et al. (2013) | United States, Israel | Substance use | Computer science, psychology, and neuroscience; a reflection on what expertise was considered useful is not provided | To understand and model the role of allostasis in drug addiction. | Not reported. |
| Martín et al. (2014) | United States | Physical activity | Engineering and public health; a reflection on what expertise was considered useful is not provided. | To explore and better understand Social Cognitive Theory through dynamical systems modelling and simulation, in addition to exploring the role of habituation. | Not reported. |
| Martín et al. (2015) | United States | Physical activity | Engineering and public health; a reflection on what expertise was considered useful is not provided. | To improve understanding of the system dynamics through designing and testing input signals within an adaptive physical activity intervention. | Not reported. |

Time Authors Health behaviour Modelling purpose/ required for (year) Country Team expertise objective modelling (s) Martín et al. **United States** Physical activity Engineering and public To develop a closed-loop, Not (2016)health; a reflection on intensively adaptive reported. what expertise was intervention for physical considered useful is not activity, informed by a provided. dynamical model of Social Cognitive Theory. Martín et al. United States Physical activity Engineering, behavioural To explore the concept of Not (2020)science and public health; setting 'ambitious but reported. the authors mention that doable' daily step goals in the application of control a closed-loop physical engineering principles to activity intervention, the behavioural sciences informed by a dynamical is useful but do not model of Social Cognitive further elaborate on this. Theory. Navarro-**United States** Eating behaviour Engineering and public To improve the Not Barrientos and physical health; a reflection on understanding of reported. et al. what expertise was behavioural weight loss activity considered useful is not (2011)interventions by provided. expressing these as dynamical systems. Neuser et al. Germany Eating behaviour Psychiatry and psychology; To outline a dynamic Not (2020)a reflection on what variability model of food reported. expertise was considered intake, with a view to useful is not provided. better understanding aberrant eating behaviour. Pavel et al. **United States** Physical activity Engineering, computer To describe a Not (2016)and eating science, and behavioural computational model reported. behaviour science; a reflection on based on a dual process theoretical framework for what expertise was considered useful is not behaviour change. provided. Pirolli **United States** Physical activity Cognitive science; a To present a computational Not (2016a) reflection on what model that can explain reported. expertise was considered and predict the day-touseful is not provided. day dynamics of health behaviour change within an mHealth study and to formalise self-efficacy as a learning/memory process. Pirolli **United States** To better understand the Physical activity Cognitive science; a Not reflection on what dynamics of behaviour reported. (2016b) expertise was considered change, with a view to useful is not provided. developing algorithms that can personalise the selection and intensity of adaptive interventions. Pirolli et al. **United States** Physical activity Cognitive science; a To test predictions from a Not (2017)reflection on what computational model reported. regarding health expertise was considered behaviour goal success useful is not provided. under conditions of implementation intentions and different reminder dosing schedules. Riley et al. **United States** Physical activity Engineering, computer To develop a dynamic Not (2016)science, behavioural computational model of reported. science, and public Social Cognitive Theory. health; a reflection on

Table 1. Continued.

| Table ' | 1. | Continued. |
|---------|----|------------|
|---------|----|------------|

| Authors (year) | Country | Health behaviour (s) | Team expertise | Modelling purpose/ objective | Time required for modelling |
|-------------------------|---------------|-------------------------|---|---|-----------------------------------|
| | | | what expertise was considered useful is not provided. | | |
| Timms et al. (2013b) | United States | Cigarette smoking | Engineering, medicine, and public health; a reflection on what expertise was considered useful is not provided. | To develop a dynamical systems model that describes smoking behaviour change during cessation as a self- regulatory process. | Not reported. |
| Timms et al. (2014) | United States | Cigarette smoking | Engineering, medicine, and public health; a reflection on what expertise was considered useful is not provided. | To describe the process of behaviour change during a smoking cessation attempt. | Not reported. |
| Timms et al. (2013a) | United States | Cigarette smoking | Engineering, medicine, and public health; a reflection on what expertise was considered useful is not provided. | To better understand smoking cessation as a self-regulation process. | Not reported. |

when modelling complex systems and that control engineering principles can be usefully applied to the behavioural sciences.

The purpose of the modelling efforts could be broadly categorised as 'understanding dynamic processes that influence health behaviours' (20/29; 69.0%) and 'developing an adaptive intervention' (9/29; 31.0%). None of the included studies reported the time required for the interdisciplinary teams to complete their modelling efforts (0/29; 0.0%).

Modelling methods

Only one of the included studies (1/29; 3.4%) reported actively involving stakeholders in the modelling process, with personal trainers consulted to help specify an 'exercise difficulty' parameter (see Table 2). Most studies (25/29; 86.2%) drew solely on theory to identify the model components and structure. A minority of studies drew on clinical expertise within the project team and observed statistical patterns from prior work (2/29; 6.9%) or observed statistical patterns only (2/29; 6.9%). The three most commonly formalised theories were: the Social Cognitive Theory (9/29; 31.0%) (Bandura, 1986), the Self-Regulation Theory (5/29; 17.2%) (Carver & Scheier, 1998), and the Theory of Planned Behaviour (4/29; 13.8%) (Ajzen, 1991).

A minority of studies explicitly mentioned taking an iterative approach to the model development and validation process (4/29; 13.8%), with two studies providing further details. In these studies, iteration involved the formulation of an initial model structure, simulation, comparing the simulated against the empirical data, which was followed by model refinement.

With regards to internal consistency checks, most studies simulated data from their model (21/29; 72.4%). However, only a minority of studies described the simulated participant characteristics (e.g., their expected age, gender, or health behaviour profile; 7/29; 24.1%), any pre-specified simulation benchmark(s) (i.e., qualitative or quantitative patterns that the model was expected to reproduce, such as the different stages of addiction; 5/29; 17.2%), or any sensitivity checks on the parameter values or other model assumptions (e.g., whether the qualitative or quantitative model outputs remained robust across a range of parameter values; 4/29; 13.8%).

With regards to external consistency checks, many studies fit their model to real-world data from intensive longitudinal study designs and calculated goodness-of-fit statistics, such as the residual sum of squares or the percentage of fit between the data and the model output (12/29; 41.4%).

| Authors | Stakeholder | Method for identifying model | | | |
|------------------------|---------------|---|---|--|---|
| (year) | involvement | components and structure | Internal consistency checks | External consistency checks | The use of iterative practices |
| Banks et al. (2014) | Not reported. | Clinical practice and observed statistical patterns (i.e., prior clinical knowledge within the project team from substance use therapy and intensive longitudinal data from a clinical trial). | Simulation was merged with model fitting to empirical data in a type of iterative simulation-based sensitivity analysis, and therefore assumed the same participant characteristics as the empirical data. This involved selecting the initial parameter values, manually adjusting these, and observing the effects on the solution as compared with the empirical data. | Although data were simulated from two models, manual adjustment of parameter values was performed through iterative comparison with the real-world data. Participant data were collected from 89 adult drinkers with an alcohol use disorder who wanted to reduce their drinking. Participants were asked to complete daily interactive voice recordings for eight weeks. Two 'model subjects' were selected for the dynamical systems modelling based on observing their change trajectories over time and selecting individuals with interesting/prototypical patterns (i.e., subject 1 was selected because their drinking had changed in a seemingly systematic way and subject 2 because their drinking data displayed a clear and consistent downward trend). Model comparison was used to determine whether more complex versions of the two models, compared with simpler models without specific parameters, resulted in a statistically significant improvement in model fit to data, | A type of iterative simulation-based sensitivity analysis was used. This involved selecting the initial parameter values, manually adjusting these, and observing the effects on the solution as compared with the empirical data. |
| Banks et al. (2017) | Not reported. | Clinical practice and observed statistical patterns (i.e., prior clinical knowledge within the project team from substance use therapy and intensive longitudinal data from a clinical trial). | Not reported. | using the residual sum of squares. The model was fit to real-world data. Data were collected from 200 adult, problem drinking men who have sex with men. Participants were randomised into one of four treatment groups: naltrexone (NTX) and modified behavioural self-control therapy (MBSCT), NTX only, MBSCT only, or placebo. The treatment was | An iterative modelling approach was used. First, a psychological hypothesis was proposed through a preliminary model formulation. Data were simulated from the preliminary model, and the results were compared against the clinical data. This led to an improved understanding of the relationships |

Table 2. Modelling methods in the included studies.

| Table 2. Conti | fable 2. Continued. | | | | |
|-------------------|----------------------------|--|-----------------------------|---|---|
| Authors (year) | Stakeholder involvement | Method for identifying model components and structure | Internal consistency checks | External consistency checks | The use of iterative practices |
| Baretta et al. 1 | Not reported. | Theory (i.e., Self-Efficacy Theory). | Not reported. | delivered for 12 weeks, during which participants were asked to respond to daily ecological momentary assessments. A 'model subject' was selected for the dynamical systems modelling based on the following: latent-class growth analysis was used to determine cohorts based on the change in alcohol consumption over the treatment period. The cohort with the largest reduction was then selected. From this cohort, a prototypical participant was selected. Parameter estimation was performed through inverse problem methodology (i.e., the <i>fmincon</i> function in MATLAB). Data were subsequently simulated from the model with the optimal parameter values and compared with the empirical data. An 'optimal profile' was generated by | among the variables. The cycle was repeated by proposing a revised model, which incorporated the new psychological understanding. The revised model solutions more accurately reflected the dynamics in the data compared with the preliminary model, which suggested that the revised model captured the relationships among the variables better. |
| (2019) | in the ported. | fileory (i.e., self Encacy fileory). | ive reported. | the researchers, reflecting progression towards a long-term behavioural goal. Data were collected from 60 adult participants, who were asked to use the app with the embedded computational model for a period of eight weeks. The empirical data were subsequently compared against the optimal profile and participants were clustered into four behavioural subtypes (i.e., static, complicated, slow but gradual, and capable). | |

| Berardi et al. (2018) | Not reported. | Theory (i.e., Behaviour Shaping/ Operant Conditioning). | Data were simulated from the model, Not reported. first varying the parameter values, and subsequently running more targeted 'computational experiments' to examine the role of two specific parameters. The characteristics of the simulated participants were not described. No benchmarks for the simulations were specified. Sensitivity checks on the parameter values were not | Not reported. |
|------------------------------|---------------|--|---|--|
| Bobashev et al. (2017) | Not reported. | Theory (i.e., Control Theory, Allostasis Theory, and Opponent-Process Theory). | explicitly mentioned. B Data were simulated from the model, Not reported. with parameter values calibrated to produce a steady state of smoking approximately one pack of cigarettes per day. Sensitivity checks on the parameter values were not explicitly mentioned. The model was calibrated to the following typical participant: the participant starts smoking seven cigarettes per day and over a period of nine months progresses to smoking a pack a day. The participant was assumed to have unrestricted access to cigarettes during the day, except for eight hours at night during sleep. Two simulation scenarios were subsequently tested: (1) access to cigarettes was restricted for a short period of time; and (2) access to cigarettes was restricted for a longer time period. Neither sensitivity checks nor benchmarks for the simulations were explicitly mentioned | Not reported. |
| Caselles et al. (2010) | Not reported. | Theory (i.e., Unique Personality Trait Theory). | Data were simulated from the model, Not reported. with parameter values manually adjusted. The characteristics of the simulated participants were not described. Sensitivity checks on the | The model structure was obtained after 'a long trial and error process'; however, further details about the iterative process are not provided. |

| Authors (year) | Stakeholder involvement | Method for identifying model components and structure | Internal consistency checks | External consistency checks | The use of iterative practices |
|--------------------------------|----------------------------|--|--|-----------------------------|---|
| <u>v · · /</u> | | | parameter values were not explicitly mentioned. The simulations were used to examine if the model could reproduce three 'classical phases' of the addictive process (i.e., sensitisation, habituation, and return) and the ways in which personality influences and is influenced by this process (i.e., these were the simulation hanchmarks) | | |
| Dong et al. (2012) | Not reported. | Theory (i.e., Theory of Energy Balance the Theory of Planned Behaviour, and Self-Regulation Theory). | were the simulation benchmarks): , Data were simulated from the model I under conditions of no intervention and with an intervention, with manually selected parameter values. The simulations assumed a 32-year-old pregnant woman with pregravid parameters of height and weight which placed her in the overweight BMI category. Sensitivity checks on the parameter values were not explicitly mentioned. No benchmarks for the simulations were specified | Not reported. | Not reported. |
| El Mistiri et al. (2022) | Not reported. | Theory (i.e., Social Cognitive Theory). | Data were simulated from the model I under conditions of an adherent and a non-adherent participant. The simulations assumed inactive participants with 2,000 steps/day at baseline. It is unclear how parameter values were selected. Sensitivity checks on the parameter values were not explicitly mentioned. No benchmarks for the simulations were specified | Not reported. | The process of input signal design i 'iterative by nature'; however, further details about the iterative process are not provided. |
| Ghosh (2015 |) Not reported. | Theory (i.e., The Fogg Behaviour Model). | The computational feasibility (e.g., simulation run time) of the model was evaluated through test simulations and a series of logical queries, checking that the number of states were reasonable for future model simulations and applications. The characteristics of the simulated participants were not described. | Not reported. | Not reported. |

| Giraldo et al. Not reported. (2017a) | Theory (i.e., Lewin's Theory of Group Dynamics) and observed statistical patterns (i.e., field data from people surveyed when visiting a bar). | Data were simulated from the model. Not reported. Some of the initial parameter values were informed by field data collected from 1,024 people surveyed at 30 different bars. The characteristics of the participants were not described. The simulations were used to gain a better understanding of how the model parameters affect the possible blood alcohol content (BAC) level trajectories that can be described by the system, assuming different parameter starting values. Standard dynamical systems techniques (Lyapunov stability analysis of non- smooth systems) were used to investigate the stability of the system. No benchmarks for the simulations were specified. | Not reported. |
|---|---|---|---------------|
| Giraldo et al. Not reported. (2017b) | Observed statistical patterns (i.e., a controlled experiment to estimate blood alcohol content levels under conditions of fasting and being fed, and field data from people surveyed when visiting a bar). | Data were simulated from the model. Not reported. Initial parameter values were selected through a combination of the following: random draws from a uniform distribution; a controlled experiment with 12 participants; field data from 1,024 people surveyed at 30 different bars; and manual selection. The characteristics of the participants in the controlled experiment and the observational study were not described. The simulations were used to gain a better understanding of how the model parameters affect the possible blood alcohol content (BAC) level trajectories that can be described by the system, assuming different parameter starting values. Standard dynamical systems techniques (Lyapunov stability analysis of non-smooth systems) were used to investigate the stability of the system. No benchmarks for the simulations were specified. | Not reported. |

| Table 2. Co | ntinued. | | | | |
|-----------------------------|----------------------------|---|---|---|--------------------------------|
| Authors (year) | Stakeholder involvement | Method for identifying model components and structure | Internal consistency checks | External consistency checks | The use of iterative practices |
| Grasman et al. (2016) | Not reported. | Not reported (but the concepts of self-control and craving are at the core of the model). | Data were simulated from the model under conditions of cues and developing an addiction, repeated relapses, and a therapeutic intervention. The characteristics of the simulated participants were not described; however, the authors mention that they imagined situations in which individuals become a member of a community where customs exist that may lead to addiction, such as adolescents at the brink of the legal drinking age, or adults who enter a new peer group or start a new living in a different culture. It is unclear how the parameter values were selected. The authors report that the system behaviour was robust to changes in the parameter values, although details about the sensitivity checks were not described. No benchmarks for the simulations were specified. | Not reported. | Not reported. |
| Guastello (1984) | Not reported. | Theory (i.e., Opponent Process Theory). | Not reported. | Not reported. | Not reported. |
| Klein et al. (2013) | Not reported. | Theory (i.e., the Transtheoretical Model, Social Cognitive Theory, Self-Regulation Theory, the Theory of Planned Behaviour, Attitude Formation Theory, the Health Belief Model, and Relapse Prevention Theory). | Not reported. | Data were collected from 40 healthy adults. A second study included 14 adults with chronic conditions (i.e., cardiovascular disease and type 2 diabetes). The model was applied to the empirical data to identify 'bottlenecks' for intervention. | Not reported. |
| Levy et al. (2013) | Not reported. | Theory (i.e., The Allostatic Theory of Drug Abuse). | Data were simulated from the model under 'archetypal patterns of drug seeking', with parameter values informed by the available literature. The characteristics of the simulated participants were not described. Sensitivity checks on the parameter values were performed. No benchmarks for the simulations were specified. | Not reported. | Not reported. |

| Martín et al. (2014) | Not reported. | Theory (i.e., Social Cognitive Theory). | Data were simulated from the model under conditions of low self- efficacy, initiation of the behaviour followed by maintenance, and habituation. The characteristics of the simulated participants were not described. It is unclear how the parameter values were selected. Sensitivity checks on the parameter values were not explicitly mentioned. No benchmarks for the simulations were specified. | The model was fit to empirical data, with parameter estimation performed. Data were from a subset of participants from a larger study - i.e., 68 adults aged 45+ years who agreed to participate in an experiment with the support of a smartphone for a period of eight weeks. Data were subsequently simulated from the updated model with the optimal parameter values (i.e., following parameter estimation), and compared with the empirical data, calculating the goodness of fit. | Not reported. |
|-------------------------|---------------|---|---|---|---------------|
| Martín et al. (2015) | Not reported. | Theory (i.e., Social Cognitive Theory). | Data were simulated from the model, with parameter values selected based on a previous study. The characteristics of the simulated participants were not described. Sensitivity checks on the parameter values were not explicitly mentioned. The validity of the model was explored through specifying desired behaviour change (i.e., noisily increasing daily steps). The model parameters were then calibrated to ensure that the expected behaviour could be produced by the model. Based on this informative model, different interventions were tested to understand how a real-world participant could be intervened on to reach the desired levels of daily steps. | Not reported. | Not reported. |
| Martín et al. (2016) | Not reported. | Theory (i.e., Social Cognitive Theory). | Data were simulated from the model, with parameter values selected based on a previous study. The characteristics of the simulated participants were not described. Sensitivity checks on the parameter values were not explicitly | Not reported. | Not reported. |

| Table 2. Con | 'able 2. Continued. | | | | | | | |
|-------------------------|----------------------------|--|---|---|--------------------------------|--|--|--|
| Authors (year) | Stakeholder involvement | Method for identifying model components and structure | Internal consistency checks | External consistency checks | The use of iterative practices | | | |
| Martín et al. (2020) | Not reported. | Theory (i.e., Social Cognitive Theory). | mentioned. The validity of the model was explored through specifying desired behaviour change (i.e., noisily increasing daily steps). The model parameters were then calibrated to ensure that the expected behaviour could be produced by the model. Based on this informative model, different interventions were tested to understand how a real-world participant could be intervened on to reach the desired levels of daily steps. Data were simulated from the model. It is unclear how parameter values were selected. The characteristics of the simulated participants were not described. Sensitivity checks on the parameter values were not explicitly mentioned. No benchmarks for the simulations were specified. Next, a series of simulations were conducted to show the model's ability to produce well-known responses predicted by Social Cognitive Theory, including: conditions to identify 'ambitious but doable' goals were performed, including if the model could reproduce the 'inverted U' response to the continuous application of a positive stimulus. The system was checked for stability of solutions. | The model was fit to real-world data to N estimate the model parameters. Data were from a subset of participants from a larger study - i.e., 68 adults aged 45+ years who agreed to participate in an experiment with the support of a smartphone for a period of eight weeks. Data were subsequently simulated from the updated model with the optimal parameter values (i.e., following parameter estimation), and compared with the real-world data, calculating the goodness of fit. | lot reported. | | | |
| | | | checked for stability of solutions. | | | | | |

| Navarro- Barrientos et al. (2011) | Not reported. | Theory (i.e., Theory of Energy Balance and the Theory of Planned Behaviour). | Data were simulated from the model under conditions of understanding participant variability and optimising the intervention. Data from the Minnesota semi-starvation experiment (i.e., 32 healthy men) were used to inform the energy balance sub-model. For the full model simulations, a healthy male participant was assumed. Parameter values were partly selected based on the available literature. Sensitivity checks on the parameter values were not explicitly mentioned. No benchmarks for the simulations were specified. | Not reported. | Not reported. |
|--|---------------|--|--|--|---------------|
| Neuser et al. (2020) | Not reported. | Theory (i.e., Variable Reward Sensitivity). | Data were simulated from the model for 400 participants under conditions of high/low reward sensitivity and high/low variability (i.e., four crossed groups), with parameter values drawn from a distribution or informed by the available literature. The characteristics of the simulated participants were not described. The model was subsequently fit to the simulated data to estimate the parameters and to confirm that the intended differences in mean and variability of reward sensitivity were recovered by the model (i.e., 'parameter recovery'). Next, simulations were run to explore how variability in reward sensitivity may relate to calorie intake across multiple days. | Not reported. | Not reported. |
| Pavel et al. (2016) | Not reported. | Theory (i.e., Dual Process Theory and Learning Theory). | Not reported. | The model was fit to real-world data. Data were collected from 204 participants who spent more than 120 min/day in sedentary leisure activity, exercised less than 60 min/ | Not reported. |

| Table 2. Co | 'able 2. Continued. | | | | | | |
|--------------------|--|---|--|---|--------------------------------|--|--|
| Authors (year) | Stakeholder involvement | Method for identifying model components and structure | Internal consistency checks | External consistency checks | The use of iterative practices | | |
| Pirolli | Experts (i.e., certified | Theory (i.e., ACT-R. Social Cognitive | Data were simulated from the model. | day, consumed more than 8% of their intake energy in saturated fat, and ate less than five portions of fruits and vegetables per day. Participants were randomised into one of four treatment groups. The characteristics of the participants were not described. It is unclear what method of parameter estimation was used. Correspondence between the data simulated from the model with the optimised parameter estimates and the real-world data was visually determined. A model-tracing approach was used to | Not reported. | | |
| (2016a) | personal trainers) were asked to rate the difficulty of a range of physical exercises. | Theory, and Goal Setting Theory) and statistical patterns (i.e., an experimental study investigating the effects of adaptive daily goal assignments). | The simulations were informed by an experimental study with 65 adult participants who were randomly assigned to three conditions with different 28-day goal progressions. It is unclear how the parameter values were selected, apart from the exercise difficulty parameter values, which were selected based on a prior Rasch model that was fitted to experimental data. Sensitivity checks were performed, with no major effects on the model results. No benchmarks for the simulations were specified. | compare initial model predictions with real-world data from an experimental study with 65 adult participants (i.e., the same sample that was used to inform the model building and simulations). Next, the model was fit to the real-world data, using a non-linear least squares algorithm. This led to an improved fit compared with the model-tracing step. | | | |
| Pirolli (2016b) | Not reported. | Theory (i.e., ACT-R, Social Cognitive Theory, and Goal Setting Theory) and statistical patterns (i.e., experimental study investigating the effects of adaptive daily goal assignments). | Data were simulated from the model. I The simulations were informed by an experimental study with 65 adult participants who were randomly assigned to three conditions with different 28-day goal progressions (i.e., easy, challenging, and personalised). It is unclear how the parameter values were selected. Sensitivity checks on the parameter values were not explicitly mentioned. No benchmarks for the simulations were specified. | Not reported. | Not reported. | | |

| Pirolli et al. (2017) | Not reported. | Theory (i.e., ACT-R, the Theory of Planned Behaviour, and Habit Theory). | Not reported. | The model was fit to real-world data. Data were collected from 64 adult participants who were randomly assigned to the 10 cells of an incomplete factorial design. Parameter estimation was conducted by minimising the Brier score between model-predicted probability of success and observed success using the <i>optimx</i> R package using a quasi-Newton method (i.e., limited- memory BFSG). Correspondence between the data simulated from the model with optimised parameter estimates and the real-world data was visually determined. | Not reported. |
|--------------------------|---------------|---|--|---|---------------|
| Riley et al. (2016) | Not reported. | Theory (i.e., Social Cognitive Theory). In addition, the authors' best judgement was used as a complement due to the lack of precision of the Social Cognitive Theory. | Data were simulated from an initial model, which resulted in modifications to the parameter values. Next, data were simulated from the refined model under conditions of low and high self- efficacy. The characteristics of the simulated participants were not described. Sensitivity checks using different parameter values were mentioned but no details were provided. The model behaved consistent with theory, with weaker effects of cues under conditions of low self-efficacy and stronger effects under conditions of high self- efficacy (i.e., these were the simulation benchmarks). | Not reported. | Not reported. |
| Timms et al. (2013) | Not reported. | Theory (i.e., Self-Regulation Theory). | Simulations were conducted for a new, hypothetical intervention compared with no intervention. The simulations were informed by data from 403 participants who were assigned to one of four treatment options in a clinical trial. No further details of the participant characteristics were provided. No benchmarks for the simulations were specified. | The model was fit to real-world data, with parameter estimation performed through a prediction-error minimisation algorithm. Data were collected from 403 participants who were assigned to one of four treatment options in a clinical trial. No further details of the participant characteristics were provided. Goodness of fit statistics were calculated. | Not reported. |

| Authors (year) | Stakeholder involvement | Method for identifying model components and structure | Internal consistency checks | External consistency checks | The use of iterative practices |
|------------------------|----------------------------|--|-----------------------------|---|--------------------------------|
| Timms et al. (2014) | Not reported. | Theory (i.e., Self-Regulation Theory). | Not reported. | The model was fit to real-world data, with parameter estimation performed through a prediction-error minimisation algorithm. Data were collected from 403 participants who were assigned to one of four treatment options in a clinical trial. No further details of the participant characteristics were provided. Goodness of fit statistics were calculated. | Not reported. |
| Timms et al. (2013) | Not reported. | Theory (i.e., Self-Regulation Theory). | Not reported. | The model was fit to real-world data, with parameter estimation performed through a prediction-error minimisation algorithm. Data were collected from 403 participants who were assigned to one of four treatment options in a clinical trial. This study focuses on one active treatment and the no treatment control arm. In the active treatment group, 100 participants received both active bupropion and counselling: 46.0% female; 1.0% Hispanic, 90.0% White, 7.0% Black, and 3.0% other; mean age, 36.9 ± 11.5 years; mean baseline Fagerström Test for Nicotine Dependence score, 5.0 ± 2.5. In the no treatment control group, 100 participants received a placebo drug: 54.0% female; 0.0% Hispanic, 92.0% White, 5.0% Black, and 3.0% other; mean age, 39.2 ± 11.4 years; mean baseline score, 5.1 ± 2.1. Goodness of fit statistics were calculated. | Not reported. |

Table 2. Continued.

However, just over a third of studies described the participant characteristics in the real-world studies (10/29; 34.5%). Only one study reported that any model comparisons (i.e., the comparison of goodness-of-fit statistics for multiple model versions against the empirical data) had been made (1/29; 3.4%).

Model reporting

The model reporting is described in Table 3. The most frequently used mathematical formalisms/ frameworks were differential equations (17/29; 58.6%) or difference equations (7/29; 24.1%), with a minority of studies (4/29; 13.8%) using formalisms categorised as 'other' (e.g., Bayesian dynamic networks, cusp catastrophe models). Differential equations represent the relationship between one or more changing quantities (e.g., self-efficacy) with respect to another quantity (e.g., time). Differential equations are closely related to difference equations; the former represent continuous time, and the latter represent discrete time (i.e., separate time points). The studies using differential equations typically embedded these within a broader control systems or fluid dynamics framework, which, for example, assume the fundamental physical principles of the conservation of mass and energy. In contrast, mathematical frameworks such as Bayesian dynamic networks do not make such assumptions. The software used to implement the models was most frequently not reported (13/29; 44.8%), followed by MATLAB (9/29; 31.0%), R (3/29; 10.3%), or software that was categorised as 'other' (4/29; 13.8%).

The most commonly reported model time step was daily, with models describing changes from one day to the next (17/29; 58.6%); however, the model time steps in the remaining studies ranged from minute-to-minute to weekly. The model run lengths (i.e., the total length of time the model was set to run to observe its behaviour) varied widely, from six hours to 500 weeks. Most studies did not provide a rationale for the selected model time steps or run length (17/29; 58.6%), with the remaining studies referring to the availability of data from prior work or arguing that the health behaviour of interest fluctuates at the specified frequency (12/29; 41.4%).

A schematic of or table with the model variables and free parameters (i.e., a comprehensive summary of the model itself) was provided in most studies (23/29; 79.3%). The models varied widely in complexity, with the approximate count of the number of model variables and free parameters ranging from three to 30. The type of variables and free parameters included in the models were aligned with the formalised theories. For example, the models grounded in the Social Cognitive Theory included variables such as 'self-efficacy' and 'outcome expectations', while the models grounded in the Theory of Planned Behaviour included variables such as 'intention' and 'perceived behavioural control'. Code or pseudo-code was publicly available only in a minority of studies (3/29; 10.3%).

The outcomes of the modelling efforts (see Table 3) could be broadly categorised into 'dynamic processes were better understood' (22/29; 75.9%), 'the efforts can be used to inform future intervention development' (17/29; 58.6%), 'calibration against real-world data is needed' (9/29; 31.0%), and 'practical modelling challenges were articulated, including those relating to the data collection, model implementation, or computational requirements' (6/29; 20.7%).

Discussion

Principal findings

This scoping review aimed to provide an overview of formal, dynamical systems models of health psychology theories unfolding at the within-person level. Formal, dynamical systems modelling is a promising method which stands to (at least partly) counteract the theory crisis in psychology and beyond. We sought to probe the existing literature on this topic to summarise the characteristics and purposes of current modelling efforts in the health psychology domain. In addition, we aimed to

| Authors (year) | Mathematical formalisms and software | Model steps and run length | Model reporting | Model summary | Modelling outcomes/what was learnt |
|--------------------------|--|---|---|--|--|
| Banks et al. (2014) | Differential equations; software not reported. | The model steps (triweekly) and run length (eight weeks) were selected due to the availability of data from a clinical trial (run length) and following inspection of meaningful data patterns (model steps), which indicated that a triweekly rather than daily timescale would be most suitable for observing trends in alcohol consumption (i.e., the daily data had too many fluctuations). | Schematics of the model components/parameters and structure for two individuals are provided (approximate count of model components: 6). Strong relationships are depicted by solid lines and weak relationships by dashed lines. Code/pseudo-code is not publicly available. | Different dynamical models were generated for the two 'model subjects'. Model 1: Number of drinks consumed, limit, commitment to quit, desire to drink, guilt (shorthand for norm violation), and weight parameters. Model 2: Number of drinks consumed, mood, commitment, desire to drink, guilt, pleasant events, and weight parameters. | Developing dynamical models of complex systems is an iterative process. Usual regression methodologies which involve averaging responses over several individuals/questions are inferior when it comes to understanding the behavioural mechanisms of change in alcohol use. The way data are usually collected presented some issues when developing a formal, dynamical systems model of alcohol use/behaviour change. |
| Banks et al. (2017) | Differential equations; MATLAB. | No rationale is provided for the model steps (daily) or run length (12 weeks). | A schematic of the model components/parameters and structure is provided (approximate count of model components: 7). Code/pseudo-code is not publicly available. | Number of drinks consumed, norm violation, confidence, commitment, personal norm, desire to drink, weight parameters. | The method and results illustrate a preliminary proof-of-concept for using within-person dynamical systems modelling in research investigating behaviour change. However, there are difficulties in pursuing quantitative dynamic modelling with Likert scale data. Developing dynamical models is an iterative process, and the revised model (compared with the preliminary model) better captured the relationships among the variables. |
| Baretta et al. (2019) | Dynamic decision network; software not reported. | No rationale is provided for the model steps (weekly) or run length (eight weeks). | A schematic of the model components/parameters and structure is provided (approximate count of model components: 4). Code/pseudo-code is not publicly available. | Goal, behaviour, self-efficacy, and factors external to the training. | A mathematical description of a behaviour change model based on self-efficacy theory and adaptive goal setting is presented, which requires tuning to real-world data. |
| Berardi et al. (2018) | Difference equations; MATLAB. | No rationale is provided for the model steps/run length (250 unspecified time units). | A schematic of the model components/parameters and structure is provided (approximate count of model components: 7). Code/pseudo-code is not publicly available. | Range of behaviours, target behaviour class, number of behaviours in repertoire, fitness function (reinforcement strength), cloning, proportion mutated, mutation, and scaling parameters. | This work demonstrates the viability of using computational models to investigate behaviour shaping routines. The results indicate that shaping was effective at engendering higher levels of the target behaviour compared with when only the target behaviour |

Table 3. Model reporting in the included studies.

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| Bobashev et al. (2017) | Differential equations; R and Java. | No rationale is provided for the model steps (hours and days) or run length (17 to 90 days). | A schematic of the model components/parameters and structure is provided (approximate count of model components: 14). Code/pseudo-code is not publicly available. | Effect of the drug, accumulation of the drug/toxicity, habit, long-term consumption, long-term hedonistic memory, trigger that prompts self- administration, binge/intoxication, stressors, external cues, availability of cigarettes, withdrawal, craving, scaling parameters, and threshold parameters. | real-world scenarios may present challenges. A multiscale simulation model of drug self-administration was developed. Implementing this simple model yielded insights that were interpreted as important (e.g., 'the feeling of craving will eventually subside if the subject stays abstinent for long enough'). The results of the simulations are as good as the model assumptions, of which there are many. There are several avenues for expanding the model, and in doing so, simulating data can provide a translational link between animals and humans. |
|------------------------------|---|--|--|--|--|
| Caselles et al. (2010) | Differential equations; Visual Basic in the SIGEM system. | No rationale is provided for the model steps (minutes) or run length (unclear). | A schematic of and table with the model components/parameters and structure are provided; however, there are some inconsistencies between these (approximate count of model components: 30). Code/pseudo- code is not publicly available. | Drug unit dose, resistance time, delay reducing rate, absorption rate constant, elimination rate constant, tonic or basal activation level, homeostatic control rate, rate of increase of the excitation effect power, rate of decrease of the excitation effect power, rate of increase of the inhibitor effect power, rate of decrease of the inhibitor effect power, consumption rate, absorption rate, ingested an non-absorbed drug, elimination rate, drug level in the body, activator effect, homeostatic control, excitation effect, inhibitor effect, excitation-inhibitor balance, activation level, extraversion, increase of the excitation effect power, reduction of the excitation effect power, excitation effect power, reduction of the inhibitor effect power, and inhibitor effect power. | A dynamic mathematical model of a stimulant (cocaine) drug addiction is presented. The model can, via simulations, reproduce expected short- and long-term dynamics and can help explain the interaction between personality and addiction. |

(Continued)

class is reinforced. The translation to

| Table 3. Con | itinued. | | | | |
|--------------------------------|--|---|---|---|--|
| Authors (year) | Mathematical formalisms and software | Model steps and run length | Model reporting | Model summary | Modelling outcomes/what was learnt |
| Dong et al. (2012) | Differential equations; software not reported. | The model steps (daily) and run length (40+ weeks of pregnancy) were selected because physical activity and energy intake guidelines operate at the daily level and the total duration of pregnancy is ~40 weeks. | Schematics of the model components/parameters and structure are provided (approximate count of model components: 19). Code/pseudo- code is not publicly available. | Behaviour, intention, attitude towards the behaviour, subjective norm, perceived behavioural control, behavioural belief, evaluation of outcome, normative belief, motivation to comply, control belief, power of control belief, goal, self- regulatory controller, fat-free mass, fat mass, energy intake, energy expenditure, weights, and disturbances. | A dynamical model which can be used to underpin a behavioural intervention to control gestational weight gain is proposed. |
| El Mistiri et al. (2022) | Differential equations; software not reported. | The model steps (within-day and day- to-day) and run length (260 days, split into 10 cycles) were selected as such a design was expected to be required for eliciting transient responses (i.e., system responses to a change from an equilibrium). | A schematic of the model components/parameters and structure is provided; however, the final model contains added/ removed elements (approximate count of model components: 16). Code/pseudo-code is not publicly available. | Behavioural outcome, behaviour, outcome expectancy, self-efficacy, cue to action, perceived barriers/ obstacles, environmental context, goal setting, inspiring bouts (i.e., a categorical four level input signal combining a pseudo-random binary sequence with a random multi-level sequence), availability, opportunity, inflow resistances, outflow resistances, time constants, time delays, and unmeasured disturbances. | This work provides proof-of-concept of the utility of system identification approaches in input signal design for behavioural intervention experiments, focusing specifically on the selection of ideal times to deliver just-in-time adaptive interventions. |
| Ghosh (2015) | State transition model (Kripke structure); NuSVM (symbolic model checking software). | No rationale is provided for the model steps (unclear) or run length (unclear). | A schematic of the model components/parameters and structure is provided (approximate count of model components: 5). Code/pseudo-code is not publicly available. | Behaviour, state, motivation, ability, and trigger. | This work formalises a possible set of persuasive actions for wellbeing. The formalisation was applied to smoking cessation as a proof-of- concept case study. |
| Giraldo et al. (2017a) | Differential equations; MATLAB. | No rationale is provided for the model steps (hours) or run length (four hours). | A schematic of the model components/parameters and structure is provided (approximate count of model components: 9). Code is available. | Blood alcohol content (BAC), BAC rate of change, alcohol intake, perception of BAC rate of change, BAC acceleration, desired effect, neighbour's BAC, environmental bias, and scaling parameters. | The model provides a framework for studying the effect of social processes on individual alcohol intake during a drinking event. This paper illustrates how field data and computational and mathematical modelling complement each other. As part of the iterative modelling process, these efforts will help refine future field studies. |

| Giraldo et al. (2017b) | Differential equations; MATLAB. | The model steps (minutes) and run length (six hours) were selected based on research focused on the pharmacokinetics of alcohol. | No schematic of or table with the model components/parameters and structure is provided (approximate count of model components: 7). Code is available. | Blood alcohol content (BAC), BAC rate of change, alcohol intake, subjective intoxication, desired level of intoxication, metabolism, and scaling parameters. | The model was developed to characterise the BAC dynamics of an individual during a drinking event. The results provide useful insights into the mechanisms that drive the decision-making process during drinking events. Additional real- time drinking event data that includes individual, group, and environmental level variables will help validate and update hypotheses about drinking event dynamics. |
|-----------------------------|--|---|---|--|--|
| Grasman et al. (2016) | Difference equations; Microsoft Excel. | The model steps (weekly) were selected based on the authors' assumption that lifestyle behaviours exhibit cyclic patterns with a periodicity of one week (although no reference was provided for this). No rationale is provided for the run length (500 weeks). | A schematic of the model components/parameters and structure is provided (approximate count of model components: 9). Code/pseudo-code is not publicly available. | Acting out, external forces, self-control, craving, vulnerability, impact, decay, maximum capacity, and constants. | Not reported. |
| Guastello (1984) | Cusp catastrophe model; software not reported. | No rationale is provided for the model steps (unclear) or run length (unclear). | No schematic of or table with the model components/parameters and structure is provided (approximate count of model components: 5). Code/pseudo- code is not publicly available. | Drug use, social support, dosage, drug history, and availability. | Addiction and withdrawal can be considered part of the same process. |
| Klein et al. (2013) | Discrete maths/ threshold model; bespoke software. | No rationale is provided for the model steps (unclear) or run length (unclear). | A schematic of the model components/parameters and structure is provided (approximate count of model components: 22). Pseudo-code is available. | Susceptibility, severity, pros/cons, emotions, social norms, barriers, skills, cues, threat, attitude, self- efficacy, coping strategies, mood, high-risk situations, awareness, motivation, commitment, stage of change, threshold, lifetime, age, and bottleneck. | Preliminary results demonstrate the model's ability to help the digital system perform intelligent reasoning and intervene as needed, although further validation efforts are needed. |
| Levy et al. (2013) | Difference equations; MATLAB. | No rationale is provided for the model steps (multiple: minutes and hours) and run length (160 days). | A schematic of the model components/parameters and structure is provided (approximate count of model components: 18). Code/pseudo-code is not publicly available. | Mood, drug intake, drug concentration in the brain, reward set point, baseline reward threshold, lowering effect on reward threshold, cognitive state, rationality density, cognitive weights, healing intervention, stress, pain, drug craving, saliency to drug | This multiscale computational model promotes the identification of plausible hypotheses which, if experimentally tested, could provide knowledge to further improve the computational model. |

| Authors (year) | Mathematical formalisms and software | Model steps and run length | Model reporting | Model summary | Modelling outcomes/what was learnt |
|-------------------------|--|---|--|--|--|
| | | · · · | | cues, acute shock, acute trauma, acute drug priming, and acute drug cue. | |
| Martín et al. (2014) | Differential equations; MATLAB. | No rationale is provided for the model steps (daily) and run length (20 days). | A schematic of the model components/parameters and structure is provided (approximate count of model components: 13). Code/pseudo-code is not publicly available. | Behavioural outcome, behaviour, outcome expectancy, self-efficacy, cue to action, self-management skills, skills training/social persuasion, observed behaviour/vicarious learning, perceived social support/ persuasion, perceived barriers/ obstacles, intrapersonal states, internal cues, external cues, environmental context, inflow resistances, outflow resistances, time constants, time delays, and unmeasured disturbances. | This paper describes a dynamical system model of Social Cognitive Theory and illustrates how control systems engineering principles provide a promising approach for advancing health behaviour theory development (e.g., by better specifying implicit assumptions made within the Social Cognitive Theory) and for guiding the design of more potent interventions. The model also shows that habituation may have an impact on behaviour change dynamics, thus demonstrating its importance within models of Social Cognitive Theory. |
| Martín et al. (2015) | Differential equations; MATLAB. | The model steps (daily) and run length (273 days) were selected to obtain sufficient simulated data for analysis. | A schematic of the model components/parameters and structure is provided (approximate count of model components: 13). Code/pseudo-code is not publicly available. | Behavioural outcome, behaviour, outcome expectancy, cue to action, outcome expectancy for reinforcement, external cues, reinforcement, environmental context, inflow resistances, outflow resistances, time constants, time delays, and unmeasured disturbances. | The study demonstrated that through building onto a dynamical model of Social Cognitive Theory, it was possible to design a set of simulated interventions that increased physical activity in a realistic way. |
| Martín et al. (2016) | Differential equations; MATLAB. | No rationale is provided for the model steps (daily) and run length (273 days/160 days). | A schematic of the model components/parameters and structure is provided (approximate count of model components: 15). Code/pseudo-code is not publicly available. | Behavioural outcome, behaviour, outcome expectancy, expected points, cue to action, internal cues, external cues, self-efficacy, goal attainment, environmental context, inflow resistances, outflow resistances, time constants, time delays, and unmeasured disturbances. | The study demonstrated that through building onto a dynamical model of Social Cognitive Theory, it was possible to design a set of simulated interventions that increased physical activity in a realistic way. |

Table 3. Continued.

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| Martín et al. (2020) | Differential equations; MATLAB. | No rationale is provided for the model steps (daily) and run length (20 days). | A schematic of and table with the model components/parameters and structure is provided (approximate count of model components: 20). Code/pseudo- code is not publicly available. | Behavioural outcome, behaviour, outcome expectancy, self-efficacy, cue to action, self-management skills, skills training/social persuasion, observed behaviour/vicarious learning, perceived social support/ persuasion, perceived barriers/ obstacles, intrapersonal states, internal cues, external cues, environmental context, inflow resistances, outflow resistances, time constants, time delays, and unmeasured disturbances. | This paper described how Social Cognitive Theory can be represented as a dynamical system that can be used to design controllers, with the ultimate goal of improving intensively adaptive interventions in mHealth. |
|--|--|---|--|--|---|
| Navarro- Barrientos et al. (2011) | Differential equations; software not reported. | The model steps (daily) and run length (180) were partly informed by a well- known experimental study (i.e., the Minnesota semi-starvation experiment). | A schematic of the model components/parameters and structure is provided (approximate count of model components: 20). Code/pseudo-code is not publicly available. | Behaviour, intention, attitude towards the behaviour, subjective norm, perceived behavioural control, behavioural belief, evaluation of outcome, normative belief, motivation to comply, control belief, power of control belief, carbohydrate intake, fat intake, protein intake, sodium intake, lean mass, fat mass, extracellular fluid, weights, and disturbances. | A dynamical model for a behavioural intervention associated with weight loss and body change composition was proposed, which provides a potentially useful framework for understanding and optimising such interventions. The simulation results point to the need for data from experimental trials or observational studies that can be used to estimate parameter values in these models and validate the modelling framework. |
| Neuser et al. (2020) | Difference equations; software not reported. | No rationale is provided for the model steps/run length (30 runs of 150 experimental trials each). | No schematic of or table with the model components/parameters and structure is provided (approximate count of model components: 5). Code/pseudo- code is not publicly available. | Learning rate, reward prediction error, obtained reward, known reward magnitude for each option, and reward sensitivity. | The proposed model integrates disparate findings and leads to novel predictions in a quantitative framework. Model simulations can be used to make testable predictions about how latent variables such as reward sensitivity may guide eating behaviour in different settings. The results call for a stronger emphasis on within- person variability to improve mechanistic insights into eating disorders. |
| Pavel et al. (2016) | Difference equations; software not reported. | The model time steps (daily) and run length (200 days) were informed by | No schematic of or table with the model components/parameters and structure is provided | Goal, rate of forgetting/extinction, and rate of learning. | This paper illustrates the importance of computational predictive modelling for optimisation of |

Table 3. Continued.

| Authors | Mathematical formalisms and | | | | |
|--------------------------|--------------------------------|--|--|--|---|
| (year) | software | Model steps and run length | Model reporting | Model summary | Modelling outcomes/what was learnt |
| | | the availability of data from a clinical trial. | (approximate count of model components: 3). Code/pseudo- code is not publicly available. | | precision interventions to improve health behaviours. |
| Pirolli (2016a) | Difference equations; R. | The model steps (daily) and run length (28 days) were informed by the availability of data from an experimental study. | No schematic of the model components/parameters and structure is provided. A table is provided; however, it does not contain all model components (approximate count of model components: 10). Code/pseudo- code is not publicly available (although some pseudo-code is available for the ACT-R model component). | Behavioural goal, activities, ability, exercise difficulty, memory-based assessment of self-efficacy, memory- based assessment of intended effort, memory decay, gain, offset, and stress of the goal. | This model suggests that behaviour is influenced by self-efficacy, which follows an 'impulse' model, whereby individuals performing the behaviour of interest adds to the impulse but that this decays over time. |
| Pirolli (2016b) | Not reported. | The model steps (daily) and run length (100 days) were informed by the availability of data from an experimental study. | No schematic of the model components/parameters and structure is provided. A table is provided; however, it does not contain all model components/ parameters (approximate count of model components: 10). Code/ pseudo-code is not publicly available. | Behavioural goal, activities, ability, exercise difficulty, memory-based assessment of self-efficacy, memory- based assessment of intended effort, memory decay, gain, offset, and stress of the goal. | The computational model presented in this paper refines current psychological theories by exploring the dynamic interaction between goal difficulty, intended effort, and self-efficacy. |
| Pirolli et al. (2017) | Difference equations; R. | The model steps (daily) and run length (28 days) were informed by the availability of data from an experimental study. | No schematic but a table with the model components/parameters is provided (approximate count of model components: 11). Code/ pseudo-code is not publicly available. | Scaling parameter for the activation for predicting goal recall, weight parameter for implementation intention activation in predicting probability goal recall, weight parameter for memory activation of performing goals in predicting probability goal recall, scaling parameter for the utility of goal striving productions, weight parameter for implementation intention activation in utility of goal striving productions, weight parameter for memory activation of performing goals in utility of goal striving productions, scaling parameter for base-level activation | This paper showed that a computational model can be used to make precise quantitative predictions of physical activity goal achievement in response to implementation intentions and reminders. |

| | | | | learning, slope parameter for base- level activation learning, initial utility of new habit, utility learning rate for habit, and reward value for new habit. | |
|-------------------------|--|--|--|--|---|
| Riley et al. (2016) | Differential equations; software not reported. | No rationale is provided for the model a steps (daily) or run length (unclear; approximately 20 days). | A schematic of the model components/parameters and structure is provided (approximate count of model components: 19). Code/pseudo-code is not publicly available. | Behavioural outcome, behaviour, outcome expectancy, self-efficacy, cue to action, self-management skills, skills training/social persuasion, observed behaviour/vicarious learning, perceived social support/ persuasion, perceived barriers/ obstacles, intrapersonal states, internal cues, external cues, environmental context, inflow resistances, outflow resistances, time constants, time delays, and unmeasured disturbances. | This paper showed that an initial dynamical model generates precise and testable quantitative predictions for future intensive longitudinal research. The process of developing the model led to important insights about the system dynamics, which require further testing with empirical data. |
| Timms et al. (2013a) | Differential equations; MATLAB. | The model steps (daily) and run length (6 weeks) were informed by the availability of data from a clinical trial. | A schematic of the model components/parameters and structure is provided (approximate count of model components: 8). Code/pseudo-code is not publicly available. | Quit (i.e., whether the person has made an attempt to quit smoking or not), r (i.e., the craving set point), e (i.e., the deviation between the craving set point and the current craving), cigsmked (i.e., the total number of cigarettes smoked each day), craving, gain, time constant, and system zero. | The current model helps to conceptualise smoking cessation as a dynamical process. The model was presented as a first step towards developing an adaptive smoking cessation intervention. |
| Timms et al. (2014) | Differential equations; MATLAB. | The model steps (daily) and run length (6 weeks) were informed by the availability of data from a clinical trial. | A schematic of the model components/parameters and structure is provided (approximate count of model components: 8). Code/pseudo-code is not publicly available. | Quit (i.e., whether the person has made an attempt to quit smoking or not), rcrav (i.e., baseline craving level), e (i.e., the deviation between the baseline and the current craving level), cigsmked (i.e., the total number of cigarettes smoked each day), craving (i.e., current craving level), gain, time constant, and system zero | A dynamical systems model is presented, which focuses on the interplay between craving, self- regulation, and smoking cessation. The model can be used to develop an adaptive smoking cessation intervention. |
| Timms et al. (2013b) | Differential equations; MATLAB. | The model steps (daily) and run length (6 weeks) were informed by the availability of data from a clinical trial. The authors emphasise that this is a critical time frame for smoking cessation. | A schematic of and a table with the model components/parameters and structure are provided (approximate count of model components: 8). Code/pseudo- code is not publicly available. | Quit (i.e., whether the person has made an attempt to quit smoking or not), baseline craving level, daily craving difference, CPD (i.e., the total number of cigarettes smoked each day), current craving, gain (i.e., the | A dynamical systems model is presented, which can effectively leverage intensive longitudinal data to better understand self-regulatory processes during smoking cessation. |

Table 3. Continued.

| Authors (year) | Mathematical formalisms and software | Model steps and run length | Model reporting | Model summary | Modelling outcomes/what was learnt |
|-------------------|--|----------------------------|-----------------|---|------------------------------------|
| | | | | magnitude of change in an output variable per unit change of an input variable), time constant (i.e., the speed at which an output variable changes in response to a change in an input variable), and system zero (i.e., a negative value indicates inverse response, which refers to an output variable whose initial change is in a direction opposite to the net change). | |

Table 4. Initial expert-derived 'best practice' recommendations.

General recommendations

- Form an interdisciplinary modelling team with complementary expertise in, for example, psychology/public health and mathematics/engineering/computer science.
- Adopt Open Science practices to help researchers and practitioners better understand and examine the formal model. For
 example, make code or pseudo-code openly available to enable uptake and reuse.
- Devise strategies for checking that modelling papers have a sufficient degree of readability for health psychology and public health researchers without a technical background.

Specific recommendations

Model development

- Draw on and document diverse sources of knowledge (e.g., interdisciplinary scientific knowledge, clinical know-how, lived experience of participants, statistical patterns from observational or experimental studies) to help fill theoretical gaps pertaining to:
 - i The model components/structure and which mathematical framework/formalism to use;
 - ii The phenomenon/phenomena of interest (i.e., qualitative or quantitative patterns that the formal model should be able to reproduce);
 - iii The temporal resolution (e.g., the model time steps and run length) of the processes being formalised.
- Provide a comprehensive summary of the model variables and free parameters (including their plausible ranges) such that the formal model can be understood and replicated by another interested researcher.
- If aiming to fit the model to empirical data in a subsequent step, consider the number of free parameters in the model and potential consequences for the amount and complexity of data required.

Model evaluation - internal consistency checks

- Specify the simulation benchmark(s) by being clear on the phenomenon or phenomena of interest. If such knowledge is currently lacking, document this.
- Specify the characteristics (e.g., age, gender, health behaviour profile) of the simulated participants.
- Conduct and document systematic sensitivity checks on the parameter values and other model assumptions. For example, conduct and document model comparisons to help arbitrate between potential explanatory frameworks (e.g., can a simpler model give rise to the phenomenon of interest?).
- Document any model iterations (e.g., changes to the model components/structure) resulting from the simulations and any
 new research questions/knowledge gaps arising from this step.

Model evaluation - external consistency checks

- If within the project scope, fit the model to empirical data that match the temporal resolution of the processes being formalised, consistent with the Nyquist-Shannon Sampling Theorem.
- Specify the participant characteristics (e.g., age, gender, health behaviour profile) and explain any discrepancies with the simulated participant characteristics.
- Specify the parameter estimation technique used.
- If relevant, conduct and document model comparisons to help arbitrate between potential explanatory frameworks (e.g., does a simpler model with fewer components provide a better fit?).
- Document any model iterations (e.g., changes to the model components/structure) resulting from the model fitting stage and any new research questions/knowledge gaps arising from this step.

summarise and synthesise the methodological steps in published modelling studies, and to reflect on our synthesis to generate a set of expert-derived initial 'best practice' recommendations for health researchers who intend to use formal, dynamical systems modelling in their future work (see Table 4).

We found that formal modelling efforts in the health psychology domain thus far have been largely concentrated to a small number of interdisciplinary teams based in the United States, which is likely due to the novelty of this method within the health psychology field. Most modelling teams included a combination of psychologists/public health researchers and mathematicians/ engineers. The purpose of the modelling efforts was either to better understand dynamic processes underpinning health behaviours (i.e., theory-focused objectives) or to inform the development of an adaptive intervention (i.e., practice-focused objectives). The former objective aligned with our

expectations that formal, dynamical systems modelling can be used to accelerate the development and refinement of robust, testable theories that elucidate health behaviours and thus improve our understanding of *how* and *why* specific health behaviours fluctuate non-linearly over time and in response to a myriad of factors (e.g., contextual factors). The latter objective was also aligned with our expectations that formal, dynamical systems modelling can help accelerate the development of adaptive interventions, including 'just-in-time adaptive interventions' (Nahum-Shani et al., 2016), as these interventions require clearly formulated hypotheses about the dynamics of health behaviours and when and where real-time interventions may be helpful.

Contrary to our expectations, however, most studies did not involve stakeholders in the modelling process. This stands in contrast to recent modelling efforts in the clinical psychology field (Burger et al., 2020) in addition to a recent scoping review of system dynamics applications in addiction research, which reported that a third of included studies engaged people with lived experience or other stakeholders in the modelling process (Naumann et al., 2022). A plausible explanation for the discrepancy with our review is their inclusion of agent-based models (which were not included here). Agent-based modelling has a long-standing tradition of stakeholder involvement and often seeks to inform public health decisions (Hammond, 2015). In addition, the teams responsible for the modelling efforts reviewed here typically included researchers and health practitioners with interdisciplinary and complementary expertise, which may have reduced the perceived need to involve external stakeholders. Linked to this finding, we note that few of the included studies reported drawing on any other source of knowledge than available health psychology theories when specifying the model variables, free parameters, and structure. In some studies, the need to compensate for the lack of precision within health psychology theories was explicitly mentioned - i.e., it was argued that the available details about the theories of interest were insufficient for formulating the precise model equations (Riley et al., 2016). Drawing on diverse sources of knowledge to help fill theoretical gaps and documenting this - including lived experience of participants/ patients, practitioner know-how, and statistical patterns from observational or experimental studies – would be fruitful going forwards (Gibbs et al., 2023).

Although iteration was likely deployed in most (if not all) modelling efforts reviewed, it was typically not explicitly reported. Particularly for novices who are learning how to model, it would be useful for model development papers to describe what aspects of the model were refined at different stages and why. Most studies used simulation to examine the models' internal consistency; a smaller subset of studies progressed to fit their model to empirical data as part of external consistency checks. We found that few studies had specified any simulation benchmark(s) – i.e., qualitative or quantitative patterns that the model was expected to be able to reproduce. Without clarifying the phenomenon or set of phenomena that a formal model should be able to give rise to in simulations, it is difficult to judge its quality as an explanatory framework (i.e., does the specific model instantiation serves as an adequate causal explanation for the phenomenon of interest?). Without such simulation benchmark(s), any model instantiation can be argued to be adequate (van Dongen et al., 2024). If following up on the simulations with external consistency checks, this point is less relevant as a poor fit to data serves a similar purpose; however, not every modelling project can include external consistency checks due to limited resource, practical challenges, or ethical considerations. In addition, few studies reported conducting systematic checks on the parameter values or explicitly testing other model assumptions as part of their simulations. As astutely argued by modellers in adjacent fields, 'the need to test assumptions and not just predictions of a model can hardly be overemphasised' (Kokko, 2007). These considerations notwithstanding, as the formal modelling of health psychology theories is still in its infancy, and further work is required to specify the phenomena of interest that our theories seek to explain (van Dongen et al., 2024), we note that it is a great effort to first formalise available health psychology theories even without specifying simulation benchmarks/ the phenomenon of interest that the formal model should give rise to. Since each model requires several rounds of iteration, such benchmarks may also be iteratively specified as more knowledge about the system dynamics becomes available.

Most of the studies did not provide a rationale for the selected model time steps (e.g., day-to-day changes) or run length (e.g., the system dynamics projected over two days or 40 weeks). This is arguably at least as important as specifying the model components and structure and should closely match the phenomenon or set of phenomena of interest, consistent with the Nyquist-Shannon Sampling Theorem (i.e., when converting a continuous- to a discrete-time signal, it needs to be sampled at a rate that is at least twice the highest frequency present in the signal). For example, hourly dynamics may not be necessary for understanding infrequently performed health behaviours (e.g., cancer screening) but may be vital for modelling smoking or dietary lapse dynamics. As mentioned in the Introduction, psychological processes are expected to evolve over different time scales, from fast- (e.g., affect) to slow-evolving processes (e.g., habits, identity) (Rhodes, 2021). In addition, both technological and methodological advances mean that health behaviours can be monitored in (or near) real-time across different contexts and situations. As formal, dynamical systems models can accommodate temporal hypotheses, including different timescales, and data are available from studies conducted under a 'high-resolution measurement paradigm', we believe that clearer justifications for the selected model time steps and run lengths would greatly help the field going forwards.

The most frequently used mathematical formalisms were differential or difference equations, often embedded within the broader frameworks of control systems and fluid dynamics. For novice modellers with little experience, it is not always straightforward which mathematical framework to use, what the pros and cons are of different approaches, and what assumptions they engender (e.g., is there a preferred choice of mathematical formalism/framework for my modelling question?). Therefore, guidance as to how to select the mathematical approach would be helpful. A primer on different mathematical frameworks for modellers to consider is provided in Hanna Kokko's book 'Modelling for Field Biologists and Other Interesting People' (Kokko, 2007); however, the examples provided are not specifically geared towards health psychologists. In addition, a potential explanation for the low variability in the mathematical frameworks and formalisms applied in the reviewed studies is that, as with other areas of science, many researchers tend to apply the method (s) they know well for any problems they see or have a tendency to seek out problems that fit a particular method (Kokko, 2007). This is understandable, as things get guicker and more robust with repetition (e.g., limitations of the approach can be improved on with increased experience), and likely applies more broadly to how researchers tend to select which guantitative or gualitative method to use (c.f. 'If the only tool you have is a hammer, it is tempting to treat every problem as if it were a nail' [Maslow, 1966]). However, this can also lead to 'development inertia' – i.e., not considering a wider range of options and potentially over-looking a more suitable mathematical framework (Kokko, 2007).

Although most studies provided an overview of the model variables, free parameters, and structure, we deemed it challenging to extract more detailed information about the model inputs, model outputs, the variable ranges, and the number of free parameters. Instead, we devised a less finegrained data item – i.e., 'the approximate count of the number of model components' – to be able to summarise the model complexity. From this rather crude measure, we could glean that the models varied widely in complexity, which has consequences both for their explanatory power and the ability to fit the model to empirical data. However, due to the typically sparse model reporting in the reviewed studies, our interdisciplinary team could not extract more precise model information with an acceptable level of confidence and within our available resources. Related to the sparse model reporting, Open Science practices do not yet appear to be the norm within formal modelling efforts in the health psychology field. A small minority of studies made their code or pseudo-code publicly available, and the software used for the model implementations was typically not reported. Directly linked to the reproducibility crisis highlighted in the Introduction, if researchers do not share code, then the outputs cannot be scrutinised or reproduced by others, which in turn hinders model uptake or reuse by other researchers. For example, the 'ODD protocol' has gained traction within agent-based modelling to make model descriptions more understandable

and complete (Grimm et al., 2010). Modellers are strongly encouraged to apply Open Science practices going forwards, notably to help others who are starting from existing models and examples when embarking on new modelling initiatives. See Table 4 for our initial expert-derived 'best practice' recommendations.

Strengths and limitations

This review was strengthened by the interdisciplinary team expertise, encompassing health psychology, behavioural science, mathematics, and engineering. To our knowledge, this is the first review summarising and communicating the role of formal, dynamical systems modelling for health psychologists. Additional strengths include the pre-registration of the scoping review protocol and double checking 100% of the data extracted from the studies.

This review also has several limitations. First, due to the challenging nature of defining what constitutes formal, dynamical systems modelling, it was difficult to determine which studies were suited for inclusion in the review. To mitigate this concern, the study screening and selection process was guided by regular discussion among the interdisciplinary review team. However, it is likely that relevant studies were not identified by our searches, as indicated by the additional studies identified through reference chaining and expertise within the review team. Future reviews on this topic are encouraged to spend additional time crafting and validating the search strategy, ensuring that all known relevant sources are being captured. This should, at least in part, be facilitated by the work done in this review to clarify what constitutes formal, dynamical systems modelling. Second, the focus on health behaviours at the within-person level, rather than at the within- and between-person level, constitutes another limitation. However, as several systematic reviews have mapped out practices related to agent-based modelling, the focus on within-person processes in the present scoping review was deemed appropriate. Third, our review focused on the formalisation of health psychology theories pertaining to health behaviours (e.g., tobacco smoking, alcohol consumption). However, health psychology also encompasses theories that seek explain phenomena such as differing illness perceptions or the self-management of chronic conditions. Future reviews would therefore benefit from expanding the scope to a wider range of health psychology theories. Finally, we did not extract information about models being deterministic (i.e., they always produce the same outputs) or stochastic (i.e., there is a degree of randomness embedded in the model, leading to variability in the outputs), or what parameter estimation techniques were used; these aspects would be interesting to consider in future work.

Avenues for future research

First, although a review of published modelling studies provides a useful lay of the land (i.e., a bottom-up approach looking at existing practices in the modelling community), to accelerate the application of formal, dynamical systems modelling to mitigate the theory crisis in health psychology and beyond, it would be useful for modellers from adjacent fields to come together to produce a set of suggested 'how to model' guidelines. This would be with a view to ensuring that there is room for debate about different modelling practices, reflecting on their pros and cons and documenting these. For example, one important aspect of formal models that is rarely discussed is the relationship between the number of free parameters and the amount/complexity of data required for model fitting, which merits further consideration. Second, bespoke and accessible training courses and tutorials should be developed for health psychologists without a mathematical background to help the community adopt these methods. Third, following the lead of computational modellers in the cognitive science field, an open-ended pre-registration form for formal, dynamical systems models is lacking (Crüwell & Evans, 2021). Producing such a fit-for-purpose pre-registration form would be a fruitful avenue for future research. Fourth, as mentioned in the Introduction, formal, dynamical systems modelling can support multiscale modelling efforts to distinguish fast- and

slow-evolving psychological processes and their interrelations. However, few of the included studies explicitly considered different time scales; this should be studied in future health psychology modelling projects. Fifth, although psychological phenomena such as 'eqo-depletion' or 'the concurrence of depression and anxiety' are rather well-defined (van Dongen et al., 2024), clearly specifying the phenomena of interest under a 'high-resolution measurement paradigm' remains more elusive. For example, it might be of interest to generate an explanatory framework for why two individuals who are both motivated to stop smoking at a given point in time either end up abstinent or return to regular smoking a few weeks later. If so, a formal model might be expected to give rise to both abstinent and lapsing/relapsing system behaviour (i.e., the simulation benchmark), results from which could contribute to further refinements of powerful frameworks that explain the complex dynamics of smoking cessation and relapse and guide intervention development. This is important, particularly in the fields of psychology and public health where enhancing health and well-being is a central goal. However, further work is required to support researchers to more clearly specify the phenomena of interest that formal, dynamical systems models within health psychology should be able to reproduce and explain (van Dongen et al., 2024). Finally, we note that many of the included studies were published in mathematical or engineering journals rather than journals specifically targeting health psychologists. 'Mathematically beautiful' models can look scary to non-modellers and typically aim to advance mathematics rather than allow health psychologists and public health researchers to engage with the theoretical claims made (Kokko, 2007). However, to support the uptake of modelling practices in the health psychology community, at least a proportion of modelling papers should be written with this audience in mind. Interdisciplinary teams could, for example, devise strategies for checking that papers in progress have a sufficient degree of readability for health psychology and public health researchers. For example, as part of our ongoing project 'COM-PLAPSE', which aims to develop and validate a formal, dynamical systems model of lapses in smokers attempting to stop, we aim to provide resources and guidance on 'how to model', which will be specifically targeted to health psychologists (https://www.olgaperski.com/research/complapse) (Perski, 2024).

Conclusion

This scoping review of formal, dynamical systems models applied to health psychology theories identified a total of 17 modelling projects reported across 29 studies. We found that current health psychology modelling efforts have largely been concentrated to a small number of interdisciplinary teams in the United States. Most models aimed to better understand dynamic processes or to inform the development of adaptive interventions. Models commonly aimed to formalise the Social Cognitive Theory or the Self-Regulation Theory and varied in complexity. Few studies involved stakeholders in the modelling process or drew on Open Science practices. Formal, dynamical systems modelling – particularly if developed based on the principles of Open Science – can help health psychologists develop and refine theories, ultimately leading to a deeper understanding of the dynamic nature of many health behaviours and enabling the development of more potent interventions.

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Data availability statement

The data underpinning the analyses are provided in Tables 1–3.

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