

How computational modeling can force theory building in psychological science

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Psychology endeavors to develop theories of human capacities and behaviors based on a variety of methodologies and dependent measures. We argue that one of the most divisive factors in our field is whether researchers choose to employ computational modeling of theories (over and above data) during the scientific inference process. Modeling is undervalued, yet holds promise for advancing psychological science. The inherent demands of computational modeling guide us towards better science by forcing us to conceptually analyze, specify, and formalise intuitions which otherwise remain unexamined — what we dub “open theory”. Constraining our inference process through modeling enables us to build explanatory and predictive theories. Herein, we present scientific inference in psychology as a path function, where each step shapes the next. Computational modeling can constrain these steps, thus advancing scientific inference over and above stewardship of experimental practice (e.g., preregistration). If psychology continues to eschew computational modeling, we predict more replicability “crises” and persistent failure at coherent theory-building. This is because without formal modeling we lack open and transparent theorising. We also explain how to formalise, specify, and implement a computational model, emphasizing that the advantages of modeling can be achieved by anyone with benefit to all.

Keywords: computational model; theoretical psychology; open science; scientific inference

Challenges for scientific inference in psychological science

Psychology is a science that attempts to explain the capacities and behaviors of the human organism. This results in a wide range of research practices, from conducting behavioural and neuroscientific experiments, to clinical

work, to qualitative work. Psychology intersects with many other fields, creating interdisciplinary sub-fields across science, technology, engineering, mathematics, and the humanities. Here we focus on a distinction within psychological science that is under-discussed: the difference in explanatory force between research programmes that use formal, mathematical, and/or computational modeling, and those that do not. To wit, programmes that explicitly state and define their models and those that do not.

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We start by explaining what a computational model is, how it is built, and how formalisation is required at various steps along the way. We illustrate how specifying a model naturally results in better-specified theories, and therefore in better science. We give an example of a specified, formalised, and implemented computational model and use it to model a cartoon example where intuition is insufficient in determining a quantity. Next, we present our path model of how psychological science should be done in order to maximise the relationship between theory, specification, and data. The scientific inference process is a function from theory to data — but this function must be more than a state function to have explanatory force — it is a *path function* which must step through theory, specification, and implementation be-

fore an interpretation can have explanatory force in relation to a theory. Our path function model also enables us to evaluate claims about the process of doing psychological and cognitive science itself, pinpointing where in the path questionable ways of doing research occur, such as *p*-hacking (biasing data analysis or collection to force statistical modeling to return significant *p*-values, e.g., Head, Holman, Lanfear, Kahn, & Jennions, 2015). Finally, we believe the field needs to use modeling to address the structural problems in theory building that underlie the so-called replication “crisis” in, e.g., social psychology (see Flis, 2019). We propose a core yet overlooked component of open science that computational modeling forces scientists to carry out: *open theory*.

A fork in the path of psychological science

Psychological scientists typically ascribe to a school of thought that specifies a framework, a theoretical position, or at the least some basic hypotheses, which they then set out to test using inferential statistics (Meehl, 1967; Newell, 1973). Almost every paper in psychological science can be boiled down to introduction, methods, analysis, results, and discussion. The way we approach science is near identical: we ask nature questions by collecting data and then report *p*-values, more rarely Bayes-factors or Bayesian inference, or some qualitative measure. Computational models do not feature in the majority of psychology’s scientific endeavours. Most psychological researchers are not trained in modeling beyond constructing statistical models of their data, which are typically applicable off-the-shelf.

In contrast, a subset of researchers — formal, mathematical, or computational modelers — take a different route in the idea-to-publication pipeline. They construct models of something other than the data directly; they create semi-formalised or formalised versions of scientific theories, often creating (or least amending) their accounts along the way. A computational modeler is somebody who has the tools to be acutely aware of the assumptions and implications of the theory they are using to carry out their science. This awareness comes, ideally, from specification and formalization, but minimally, it also comes from the necessity of writing code during implementation.

Involving modeling in a research programme has the effect of necessarily changing the way the research process is structured. It changes the focus from testing hypotheses generated from an opaque idea or intuition (e.g., a theory that has likely never been written down in anything other than natural language, if that), to testing a formal model of the theory, as well as continuing to also be able to generate and test hypotheses using empirical data. Computational modeling does this by forcing scientists to explicitly document an instance of what their theory assumes, if not what their theory is. In our view, the most crucial part of the process is creating a specification — but even just creating an imple-

mentation (programming code) leverages more explicitness than going from framework to hypothesis to data collection directly.

What is a computational model? And why build one?

Let us calculate, without further ado, and see who is right (Leibniz, 1685; translated by: Wiener, 1951)

Leibniz predicted computational modeling when he envisaged a *characteristica universalis* that allows scientists to formally express theories and data (e.g., formal languages, logic, programming languages) and a *calculus ratiocinator* that computes the logical consequences of theories and data (e.g., digital computers; Cohen, 1954; Wiener, 1951). Computational modeling is the process by which a verbal description is formalised to remove ambiguity, as Leibniz correctly predicted, while also constraining the dimensions a theory can span.

In the best of possible worlds, modeling makes us think deeply about what we are going to model, (e.g., which phenomenon or capacity), in addition to any data, both before and during the creation of the model, and both before and during data collection. It can be as simple as the scientist asking: “How do we understand brain and behaviour in this context, and why?” By thinking through how to represent the data, model the experiment, scientists gain insight into the computational repercussions of their ideas, in a much deeper and explicit way than by just collecting data. By providing a transparent genealogy for where predictions, explanations, and ideas for experiments come from, the process of modeling stops us from atheoretically testing hypotheses — a core value of open science. Open theorising, in other words explicitly stating and formalising our theoretical commitments, is done by default as a function of the process.

Through modeling, even in, or especially in, failures we hone our ideas: can our theory be formally specified, and if not, why not? Thus, we may check if what we have described formally still makes sense in light of our theoretical commitments. It aids both us as researchers communicating with each other, and it aids those who may wish to apply these ideas to their work outside science in e.g., industrial or clinical settings.

One of the core properties of models is allowing us to “safely remove a theory from the brain of its author” (A. Wills, personal communication, May 19, 2020; also see Wills, O’Connell, Edmunds, & Inkster, 2017; Wills & Pothos, 2012). Thus allowing the ideas in one’s head to run on other computers. Modeling also allows us to compare models based on one theory to those based on another and compare different parameter values’ effects within a model, including damaging models in ways that would be unethical in human participants (e.g., “lesioning” artificial neural

network models, see Guest, Caso, & Cooper, 2020). When multiple theories can make sense of the present data, this is one of the only ways to dissociate between them in a formal setting (e.g., Levering, Conaway, & Kurtz, 2019, although also see Cox and Shiffrin, *in press*; Navarro, 2019; Wills and Pothos, 2012).

Now we will walk the reader through building a computational model from scratch in order to illustrate our argument, and then present a path function of research in psychology. We emphasise that often “merely” building a formal model of a problem is not enough — actually writing code to implement a computational model is required to understand the model itself.

The pizza problem

All models are wrong but some are more wrong than others. (pastiche based on: Box, 1976; Orwell, 1945)

Imagine it is Friday night, and your favourite pizzeria has a special: two 12” pizzas for the price of one 18”. Your definition of a good deal is one in which you purchase the most food. Is this a good deal?

A Twitter user, Fermat’s Library (@fermatlibrary), posted “a useful counterintuitive fact [that] one 18 inch pizza has more ‘pizza’ than two 12 inch pizzas”¹ — along with an image similar to Figure 1. The reaction to this tweet was largely surprise or disbelief; with @MarkSykes15 replying: “But two pizzas are more than one”.² Why were people taken aback?

When it comes to comparing the two options in Figure 1, though we all agree on how the area of a circle is defined, the results of the “true” model, that one 18” pizza has more surface, and therefore is more food in Figure 1, are counterintuitive. Computational modeling is able to demonstrate how one cannot always trust one’s gut. To start, one must create: *a*) a verbal description, a conceptual analysis, and/or a theory; *b*) a formal(isable) description, i.e., a specification using mathematics, pseudocode, flowcharts, etc.; and *c*) an executable implementation written in programming code (see the red area of Figure 2 for an overview of the three steps described above). This process is the cornerstone of computational modeling and by extension of modern scientific thought, enabling us to refine our gut instincts through experience.

Experience is seeing our ideas being executed by a computer, giving us the chance to “debug” scientific thinking in a very direct way. If we do not make explicit our thinking through formal modeling, and if we do not bother to execute, i.e., implement and run our specification through computational modeling, we can have massive inconsistencies in our understanding of our own model(s). We call this issue *the pizza problem*.

Herein we model the most pizza for our buck — overkill for scientific purposes, but certainly not for pedagogical ones. For any formalised specification, including that for pizza orders in Figure 1, simplifications need to be made, so we choose to represent pizzas as circles. Therefore we define the amount of food ϕ per order option i as:

$$\phi_i = N_i \pi R_i^2 \quad (1)$$

where i is the pizza order option, N is the number of pizzas in the order, and the rest is the area of a circle. We also propose a pairwise decision rule:

$$\omega(\phi_i, \phi_j) = \begin{cases} i, & \text{if } \phi_i > \phi_j \\ j, & \text{otherwise} \end{cases} \quad (2)$$

where the output of the ω function is the order with the most food.

This is the model that everybody would have claimed to be running in their heads, but they still were surprised — an expectation violation occurred — when faced with the actual results. How do we ensure we are all running the same model? We execute it on a computer that is not the human mind! To make this model computational, we move from specification to implementation (consider where we are in the path shown in Figure 2). We notice Equation 1 is not wrong but ϕ could be defined more usefully as:

$$\phi_i = \sum_{j=1}^N \pi R_j^2 \quad (3)$$

where j is the current pizza, allowing us to sum over all pizzas N within food order i .

This change allows generalisation of the model (both in the specification above and the implementation below) to account for different radii per order (i.e., in future we can compare an 11” pizza plus a 13” pizza with one 18” pizza). One possible implementation (in Python) of our pizza model looks like this:

```
import numpy as np
import math

def food(ds):
    """
    Amount of food in an order as a function
    of the diameters per pizza (eq. 3).
    """
    return (math.pi * (ds/2)**2).sum()

# Order option a in fig. 1, two 12'' pizzas:
two_pizzas = np.array([12, 12])
```

¹ Archived tweet: archive.ph/Fb66R

² Archived tweet: archive.ph/BoyRs

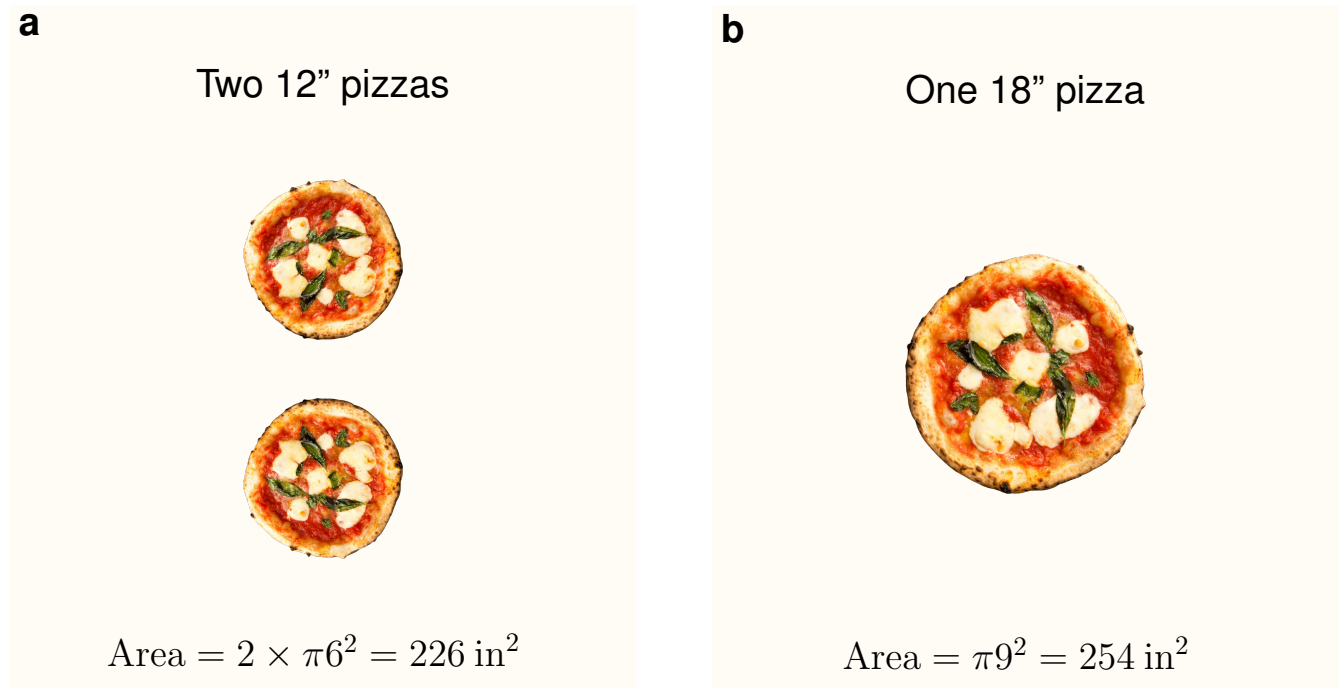


Figure 1. The pizza problem: something like comparing the two options above can appear “counterintuitive” even though we all learn the formula for the area of a circle in primary school. Compare **a**) two 12” pizzas with **b**) one 18” pizza (all three pizzas to-scale). Which order would you prefer?

```
# Option b, one 18'' pizza:
one_pizza = np.array([18])

# Decision rule (eq. 2):
print(food(two_pizzas) > food(one_pizza))
```

Importantly, this implementation change, which we choose to percolate upwards, editing our specification, does not affect the verbal description of the model. By the same token, a change in the code to use a for-loop in the definition of the `food()` function would neither affect the specification nor the theory in this case. This is a core concept to grasp: the relationships between theory, specification, and implementation — consider our “movements” up and down the path as depicted in Figure 2.

Computational modeling, when carried out the way we describe herein, is quintessentially open science: verbal descriptions of science, specifications and implementations of models are transparent, open to be replicated, and open to be modified. If one disagrees with any of the formalisms, they can plug in another decision rule or definition of the amount of food or even another aspect of the order being evaluated (e.g., perhaps they prefer more crust than overall surface). Computational modeling — when done the way we describe, since it requires the creation of specifications

and implementations — affords open theorising to go along with open data, open source code, etc. In contrast to merely stating: two 12” pizzas are more food than one 18” pizza, a computational model can be generalised and can show our work clearly. Through writing code, we debug our scientific thinking.

Model of psychological science

[T]heory takes us beyond measurement in a way which cannot be foretold *a priori*, and it does so by means of the so-called intellectual experiments which render us largely independent of the defects of the actual instruments. (p. 27 Planck, 1936)

In this section, we describe an analytical view of psychological research, shown in Figure 2. Although other such models exist for capturing some aspect of the process of psychology (e.g., Haig, 2018; Haslbeck, Ryan, Robinaugh, Waldorp, & Borsboom, 2019; Kellen, 2019; van Rooij & Baggio, 2020), ours proposes a unified account that demonstrates how computational modeling can play a radical and central role in all of psychological research.

We propose that scientific outputs can be analysed using the levels shown in the left column of Figure 2. Scientific

inquiry can be understood as a function from theory to data and back again, and this function must pass through several states to gain explanatory force. The function can express a meaningful mapping, transformation, or update between a theory at time t and that theory at time $t + 1$ as it passes through specification and implementation, which enforces a degree of formalisation. We note that each level (in blue) can, but does not have to, involve the construction of a (computational) model for that level, with examples of models shown in the left column (in green) connected by a dotted line to their associated level. If a level is not well-understood, making a model of that level helps elucidate implicit assumptions, addressing pizza problems.

A *path function* is function where the output is dependent on a path of transformations the input undergoes. Path functions are used in thermodynamics to describe heat and work transfer; an intuitive example is distance to a destination being dependent on the route and mode of transport taken. The path function moves from top to bottom in terms of dependencies, but the connections between each level and those adjacent are bidirectional (represented by large blue and small black arrows). Connections capture the adding or removing, loosening or tightening, of constraints that one level can impose on those above or below it.

In our model depicted in Figure 2, the directionality of transitions is constrained only when moving downwards. Thus, *a*) at any point transitions moving upwards are permissible — while, *b*) moving downwards is only possible if an expectation violation is resolved by first moving upwards. Downwards transitions can be thought of as functions where the input is the current layer and the output is the next. Upward transitions are more complex and involve adjusting (e.g., a theory given some data), and can involve changes to levels along the way to obtain the required (theory-)level update. With respect to why we might want to move upwards out of choice and recalling the case of the pizza model above: we updated the specification (changing Equation 1 to Equation 3) because we thought about the code/implementation more deeply and decided it is worth updating our formal specification (Equation 3). Downwards motion is not allowed if a violation occurs, e.g., our model at the current step is not inline with our expectations. Once this violation is resolved by moving to any step above, we may move downwards respecting the serial ordering of the levels. For example, when the data does not confirm the hypothesis, we must move upwards and understand why and what needs to be amended in the levels above the hypothesis. Attempting to “fix” things at the hypothesis level is hypothesising after results known (HARKing, Kerr, 1998). In the case of the pizza model, an expectation violation occurs when we realise that the one pizza is more food. At that point, we re-evaluate our unspecified/implicit model and move back up to the appropriate level to create a more sensible account.

At least implicitly, every scientific output is model- and theory-laden (i.e., contains theoretical and modeling commitments). By making these implicit models explicit via computational modeling the quality, usefulness, and verisimilitude of research programmes can be secured and ascertained. The three levels with a red background (theory, specification, and implementation in Figure 2) are those which we believe are left implicit in most of psychological research — this is especially so in parts of our field that have been most seriously affected by the so-called replication “crisis”. This tendency to ignore these levels is a result of the same process by which theory and hypothesis are conflated (Fried, 2020; Meehl, 1967; Morey, Homer, & Proulx, 2018), and by which models of the data are taken to be models of the theory: “theoretical amnesia” (Borsboom, 2013). When models of the data are seen as models of the theory potentially bizarre situations can arise — eventually forcing (sub)fields to dramatically rethink themselves (e.g., Jones & Love, 2011).

Framework

A framework is a conceptual system of building blocks for creating facsimiles of complex psychological systems, see topmost level of Figure 2. A framework is typically described using natural language and figures, but can also be implemented in code like ACT-R (Anderson & Lebiere, 1998) and Soar (Newell, 1992). Some frameworks appear superficially simple or narrow, like the concept of working memory (Baddeley, 2010) or dual-systems approaches (Dayan & Berridge, 2014; Kahneman, 2011), while others can be all-encompassing such as unified theories of cognition (Newell, 1990) or connectionism (McClelland, Rumelhart, & the PDP Research Group, 1986).

In the simplest case a framework is the context, the interpretation of the terms of a theory (Lakatos, 1976). Frameworks usually require descending further down the path before they can be computationally modeled (Hunt & Luce, 1992; Vere, 1992). While it is possible to avoid explicit frameworks, it is “awkward and unduly laborious” (Suppes, 1967, p. 58) to work without one and thus depend on the next level down in the path to do all the heavy lifting.

It is not the case that all psychological models are or can be evaluated against data directly. For example, ACT-R is certainly not: we have to descend the path first, creating a specific theory, then a specification, then an implementation, and then generate hypotheses, before any data can be collected (see Cooper, 2007; Cooper, Fox, Farrington, & Shallice, 1996).

Theory

A theory is a scientific proposition — described by a collection of natural language sentences, mathematics, logic, and figures — that introduces causal relations with the aim

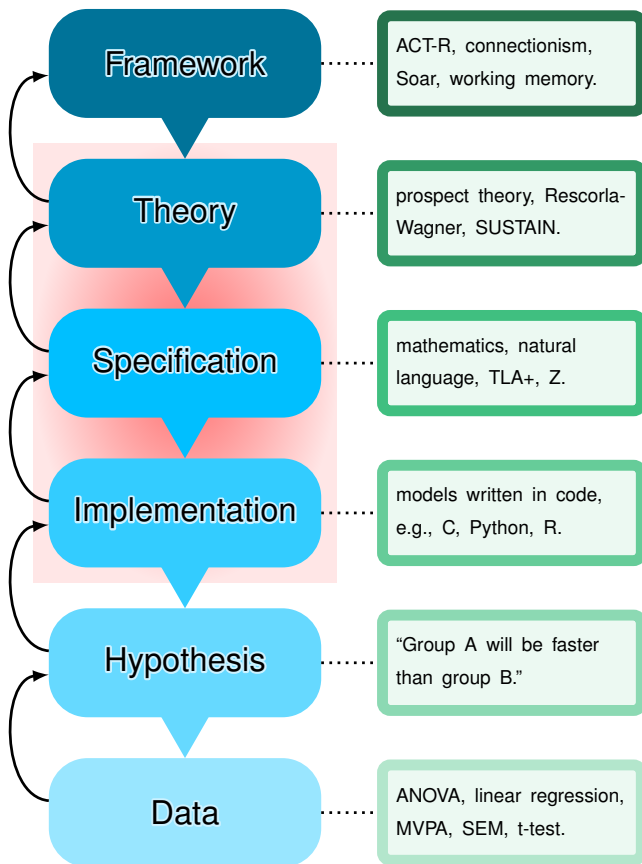


Figure 2. One of many possible paths (in blue) that can be used to understand and describe how psychological research is carried out with examples of models at each step shown on the left (in green). Each research output within psychology can be described with respect to the levels in this path. The three levels superimposed on a red background (theory, specification, implementation) are those that are most often ignored or left out from research descriptions.

of describing, explaining, and/or predicting a set of phenomena (Lakatos, 1976), see second level of Figure 2. Examples of psychological theories are prospect theory (Kahneman & Tversky, 1979), the Rescorla-Wagner model for Pavlovian conditioning (Rescorla & Wagner, 1972), and SUSTAIN, an account of categorisation (Love, Medin, & Gureckis, 2004).

To move to the next level and produce a specification for a psychological theory, we must posit a plausible mechanism for the specification model to define. As can be seen from our path, direct comparisons to data can only happen once a model is at the right level. However, not all psychological models must be (or can be) evaluated against data directly. Theoretical computational models allow us to check if our ideas, when taken to their logical conclusions, hold up (e.g.,

Guest & Love, 2017; Martin, 2016, 2020; Martin & Baggio, 2020; van Rooij, 2008). If a theory cannot lead to coherent specifications, it is our responsibility as scientists to amend, or more rarely, abandon it, in favour of one that does.

Specification

A specification is a formal(isable) description of a system to be implemented based on a theory, see third level of Figure 2. It provides a means of discriminating between theory-relevant, closer to the core claims of the theory, and theory-irrelevant, auxiliary assumptions (Cooper & Guest, 2014; Lakatos, 1976). Specifications provide both a way to check if a computational model encapsulates the theory, and a way to create a model even if the theory is not clear enough, simply by constraining the space of possible computational models. Specifications can be expressed in natural language sentences, mathematics, logic, diagrams, and formal specification languages, such as Z notation (Spivey & Abrial, 1992) and TLA+ (Lamport, 2015).

The transition to code from specification has been automated in some cases in computer science (Monperrus, Jézéquel, Champeau, & Hoeltzener, 2008). In psychology, creating an implementation typically involves taking the specification implicitly embedded in a journal article and writing code that is faithful to it. Without specifications we cannot debug our implementations, and we cannot properly test our theories (Cooper et al., 1996; Cooper & Guest, 2014; Miłkowski, Hensel, & Hohol, 2018).

Implementation

An implementation is an instantiation of a model created using anything from physical materials, e.g., a scale model of an airplane (Morgan & Morrison, 1999), to software, e.g., a git repository, see fourth level of Figure 2. A computational implementation is a codebase written in one or more programming languages, constituting a software unit and embodying a computational model. While the concept of an implementation is simple to grasp — perhaps what most psychologists think when they hear “model” — it might appear to be the hardest step. This is arguably not the case. Provided one follows the steps in Figure 2, a large proportion of the heavy lifting is done by all the previous steps.

In some senses, implementations are the most disposable and time-dependant parts of the scientific process of Figure 2. Very few programming languages stay in vogue for more than a decade, rendering code older than even a few months in extreme cases un-runnable without amendments (Cooper & Guest, 2014; Rougier et al., 2017). This is not entirely damaging to our enterprise since the core scientific components we want to evaluate are the theory and specification. If the computational model is not re-implementable given the specification, it poses serious questions for the theory (Cooper & Guest, 2014). This constitutes an expecta-

tion violation and must be addressed by moving upwards to whichever previous level can amend the issue. However, it is premature to generalise from the success or failure of one implementation if it cannot be recreated based on the specification, since we have no reason to assume it is embodying the theory. Whether code appropriately embodies a theory can only be answered by iterating through theory, specification, implementation.

Running our computational model's code, allows us to generate hypotheses. For example, if our model behaves in a certain way in a given task, e.g., it has trouble categorising some types of visual stimuli more than others, we can formulate a hypothesis to test this. Alternatively, if we already know this phenomenon occurs, computational modeling is a useful way to check that our high-level understanding does indeed so far match our observations. If our implementation displays behaviour outside what is permitted by the specification and theory, then we need to adjust something as this constitutes a violation. It might be that the theory is under-specified and this behaviour should not be permissible. In which case we might need to change both the specification and the implementation to match the theory (Cooper & Guest, 2014). Such a cycle of adjustments until the theory is captured by the code and the code is a strict subset of the theory are necessary parts of the scientific process. Loosening and tightening theory, specification, and implementation never ends — it is the essence of theory development in science.

Hypothesis

A hypothesis is a narrow testable statement, see fifth level of Figure 2. Hypotheses in psychology focus on properties of the world that can be measured and evaluated by collecting data and running inferential statistics. Any sentence that can be directly tested statistically can be a hypothesis, e.g., “the gender similarities hypothesis which states that most psychological gender differences are in the close to zero ($d \leq 0.10$) or small ($0.11 < d < 0.35$) range” (Hyde, 2005, p. 581).

Hypothesis testing is unbounded without iterating through theory, specification, implementation and creating computational models. The supervening levels constrain the space of possible hypotheses to-be-tested. Testing hypotheses in an ad hoc way — what we could dub *hypo-hacking* — is to the hypothesis layer what *p-hacking* is to the data layer (Head et al., 2015). Researchers can concoct any hypothesis and given big enough data a significant result is likely to be found when comparing, e.g., two theoretically-baseless groupings. Another way to hypo-hack is to atheoretically run pilot studies until something “works”. When research is carried out this way “losing” the significant *p*-value, e.g., due to a failure to replicate, could be enough to destroy the research programme. Any theories based on hypo-hacking will crumble if no bidirectional transitions in the path were carried out,

especially within the steps highlighted in red in Figure 2. Having built a computational account researchers can avoid the confirmation bias of hypo-hacking, which cheats the path and skips levels.

Data

Data are observations collected from the “real world” or from a computational model, see sixth level of Figure 2. Data can take on many forms in psychology, the most common being numerical values that represent variables as defined by our experimental design, e.g., reaction times, questionnaire responses, neuroimaging, etc. Most psychology undergraduate students know some basic statistical modeling techniques. Tests such as analysis of variance (ANOVA), linear regression, multivariate pattern analysis (MVPA), structural equation modeling (SEM), the t-test, and mixed-effects modeling (e.g., Davidson & Martin, 2013), are all possible inferential statistical models of datasets.

Because data is theory-laden, it can never be free from, or understood outside, the assumptions implicit in its collection (Feyerabend, 1957; Lakatos, 1976). For example, functional magnetic resonance imaging (fMRI) data rests our understanding of electromagnetism and of the blood-oxygen-level-dependent signal's association with neural activation. If any of the scientific theories that support the current interpretation of fMRI data change then the properties of the data will also change.

If the data model does not support the hypothesis (an expectation violation), this allows us with a certain confidence to reject the experimental hypothesis. This does not however give us licence to reject a theory with as much confidence. The same caution is advised in the inverse situation (Meehl, 1967). For example, a large number of studies have collected data on cognitive training over the past century and yet consensus on its efficacy is absent (Katz, Shah, & Meyer, 2018). To escape these problems and understand how data and hypothesis relate to our working theory we must ascend the path and contextualise our findings using computational modeling. These violations cannot be addressed by inventing new hypotheses that conveniently fit our data, i.e., HARK-ing, but by asking what needs to change in our theoretical understanding.

Harking back to pizza

The pizza example (purposefully chosen in part because it is simple and devoid of psychological constructs, which bias reader's opinions towards one formalism over another) can be decomposed readily into the six levels in Figure 2. At the framework level we have the concepts of pizza, food, and order because we want to compare the total amount of food per order. These are building blocks for any account which involves deciding between orders of food made up of pizzas, even if we disagree on what aspects of the order (e.g., money,

speed of delivery), or food (e.g., calories, ingredients), or pizza (e.g., crust, transportability), we will eventually formally model and empirically test.

Then at the theory level, there are essentially two theories. The original (implicit) theory T_0 that “the number of pizzas per order corresponds to the amount of food in that order” and the post hoc corrected (explicit) T_1 that “the surface areas of the pizzas per order correspond to the amount of food in that order”. To get to T_1 , we created a specification, created an implementation, and refined the specification — we shall go into exactly how this happened using the path model of Figure 2.

Before obtaining T_1 , we descended the path by going from basically framework to hypothesis (bypassing the red area completely; recall T_0 was not explicitly stated at all, let alone formalised at the beginning) to generate the very clear prediction (and thus testable hypothesis) that the order with 2 pizzas is more food than the order with 1. Because we skipped the parts of the path that required formalising our ideas (shown in red in Figure 2), we are faced with an expectation violation. We believed that 2 12” pizzas are more food than 1 18” pizza (recall Figure 1) and we also believed that the food per order is a function of the surface area of the pizzas. Therefore, we realise our own ideas about the amount of food per order are incompatible with themselves (what we dub: the pizza problem), as well as what we know about the world from other sources (imagine if we had weighed the pizzas per order, for example). Had this been a real research programme (and not a toy example), we would have descended all the way and collected empirical data on the pizzas, by e.g., weighing them. This act of collecting observations would have further solidified the existence of an expectation violation since the 2 pizzas would have been found to, e.g., have less mass. Thus falsifying both our hypothesis and indirectly T_0 .

At the point of an expectation violation, we decided to address the steps we skipped in the red area, so we move upwards to create a formal specification S_0 embodied by Equations 1 and 2. We then attempt to descend from S_0 to create an implementation I_0 , which led to refining our specification, thus creating S_1 (Equations 3 and 2). We are now fully in the throes of formal and computational modeling by cycling through the steps shown in Figure 2 in red.

Arguably — and this is one of the core points of this article — had we not ignored the steps in red and created a theory, specification, and implementation explicitly, we would have been on better footing from the start. And so it is demonstrated that applying the path model adds information to the scientific inference process. Notwithstanding, we managed to document and update our less-than-useful assumptions by going back and formally and computationally capturing our ideas. We should all strive not to ignore these vital steps by directly focusing on them, either ourselves or by making sure the literature contains this explicit formal and computational

legwork.

What our path function model offers

We have denoted the boundaries and functions of levels within the scientific inference process in psychological research — many should be familiar with similar layers of abstraction from computer science and levels of analysis from Marr and Poggio (1976). Simpler more abstract descriptions appear higher up, while more complex descriptions of psychological science are lower down the path — e.g., data is much less “compressed” as a description of an experiment than a hypothesis. Each level is a renormalisation, coarser description, of those below (DeDeo, 2018; Flack, 2012; Martin, 2020). Higher levels contain fewer exemplars than lower levels. Moving through the path of scientific inference is a form of dimensionality reduction or of coordinate transform. Not only are there often no substantive nor formalised theories for some datasets in practice (causing chaos, Forscher, 1963), but also the principle of multiple realisability (Putnam, 1967) implies that for every theory there are infinitely many possible implementations consistent with it and datasets that can be collected to test it (Blokpoel, 2018). This helps contextualise studies that show divergence in data modeling decisions given the same hypotheses (e.g., Botvinik-Nezer et al., 2020; Silberzahn et al., 2018).

Open theories (i.e., those developed explicitly, defined formally, and explored computationally, in line with Figure 2) are more robust to failures of replication of any single study they might derive some support from, due to the specific way the path has been followed in order to develop and test them. For example, if the impetus or inspiration for theory development is a single study (that is post fact found not to replicate) because we then move to the red area, refine our ideas, and then drop back down to test them again, we will avoid dependence on a single (potentially problematic) study. Failures to replicate can not only be detected but also explained and perhaps even drive theory creation as opposed to just theory rejection. Thus, building a theory explicitly as laid out in Figure 2, even if based on some hypo- and p -hacking, means once a phenomenon is detected we ascend the path and spend time formalising our account (e.g., Fried, 2020). Using the procedure described by our path model — that asks for formalisation using specifications and implementations (or indeed anything more meta than an individual study, see Head et al., 2015) — “sins” out of individual scientists’ control, such as questionable research practises (QRPs; see John, Loewenstein, & Prelec, 2012) committed by other labs or publication bias committed by the system as a whole, can be both discovered and controlled for in many cases.

Thinking about our science with reference to Figure 2 allows us to discuss and decide where in the path claims about science are being made. In other words, not just al-

lowing us to evaluate claims about the phenomena being examined, modeled, etc., but also to evaluate general claims about how we conduct research or about how not to conduct research. For example, the claim that “[s]cience is posthoc, with results, especially unexpected results, driving theory and new applications” (Shiffrin, 2018) is not incompatible with guarding against HARKing. This is because one cannot have an account of a phenomenon without having access to some data, anecdotal, observational, and/or experimental, that guides one to notice said phenomenon in the first instance.

Theories in psychology are the result of protracted thought about and experience with a human cognitive capacity. Scientists immerse ourselves in deep thought about why and how our phenomena of study behave. This basic principle of developing theories is captured in the example of Wald’s investigation into optimally (thus minimally, due to weight) armouring aircraft to ensure pilots returned safely during the Second World War (Mangel & Samaniego, 1984). Planes returned after engaging with the Nazis with a smattering of bullet holes that were distributed in a specific way: more holes were present in the fuselage than in the engines, for example. Wald explained post hoc why and how the holes were correlated to survival. Contrary to what one might expect, areas with the least holes would benefit from armour. Wald theorised that: planes in general were likely hit by bullets uniformly, unlike the planes in the dataset; aircraft hit in the engines did not make it home and so were not present in the dataset; therefore armour should be placed over the engines, the area with the fewest bullet holes. This is not HARKing — this is formal modeling. Wald moved upwards from the data (distribution of bullet holes) to a theory (survivor bias) and created an explicit formal model that could explain and predict the patterns of the bullets in planes that made it back safely. In many cases theory development involves analysis at the data level, as an inspiration or impetus, and then a lot of scientific activity within the levels: theory, specification, and implementation. This is why we do not impose any constraints on moving upwards in Figure 2, only on moving downwards.

On the other hand, our path function model allows us to pinpoint on which level QRPs are taking place and how to avoid them. Different QRPs occur at different levels, e.g., *p*-hacking at the data level, HARKing at the hypothesis level, and so on. HARKing does not resolve expectation violations that occur when the data meets the hypothesis — it is not, e.g., TARKing (theorising after results known) which is part of the scientific practice of creating modeling accounts. To retrofit a hypothesis onto a dataset does not constitute resolving a violation because this *de novo* hypothesis is not generated directly or indirectly by a theory. If we start out with a hypothesis and collect data that rejects our hypothesis, the violation has not only occurred at the hypothesis level since

the hypothesis has been generated (via the intervening levels) by the theory. This is essentially the opposite to conjuring a new hypothesis (HARKing) that only exists in the scientific literature because it has been “confirmed” by data — data collected to test a different hypothesis.

Importantly, it is at the data and hypothesis levels that preregistration and similar methods attempt to constrain science to avoid QRPs (e.g., Flis, 2019; Szollosi et al., 2019). To ensure scientific quality, however, we propose that preregistration is not enough because it only serves to constrain the data and hypothesis spaces. Researchers who wish to develop their formal account of a capacity must ascend the path, instead of, or in addition to, in addition to e.g., preregistering analysis plans. Preregistration cannot on its own evaluate theories. We cannot coherently describe and thus cannot sensibly preregister what we do not yet (formally and computationally) understand. Indeed theories can and should be computationally embodied and pitted against each other without gathering or analysing any new data. To develop, evaluate, and stress-test theories, we need theory-level constraints on and discussions about our science. Figure 2 can serve as a first step in the right direction towards such an ideal.

By the same token, our path model allows us to delineate and discuss where computational modeling itself has been compromised by QRPs occurring at the specification and implementation levels. A typical case of this is when authors report only partial results of implementing a specification of their theory, e.g., only some implementations show the required or predicted patterns of behaviour. As mentioned, the solution is to cycle within the red area of Figure 2 in order to ensure theory-, specification- and implementation-level details are indeed assigned to and described at the correct level. Failing to do that, we propose, is a type of QRP.

Computational modeling can be seen as mediating between theory and data (Morgan & Morrison, 1999; Oberauer & Lewandowsky, 2019). Asking if we can build a model of our theory allows us to understand where our theoretical understanding is lacking. Importantly, claims are typically not falsifiable — not usually directly testable at the framework or theory level — but become more so as we move downwards. We thus iterate through theory, specification, and implementation as required until we have achieved a modeling account that satisfies all the various constraints imposed by empirical data, as well as collecting empirical data based on hypotheses generated from the computational model. Is an implementation detail pivotal to a model working? Then it must be upgraded to a specification detail (Cooper et al., 1996; Cooper & Guest, 2014). *Mutatis mutandis* for details at the specification level and so on — meaning that details at every level can be upgraded (or downgraded) as required. This process is even useful in the case of “false” models, i.e., computational accounts that we do not

agree with, can still improve our understanding of phenomena (e.g., Wimsatt, 2002; Winsberg, 2006).

As mentioned, cycling through the steps in Figure 2, shines a direct light on what our theoretical commitments are in deep ways. Mathematically specifying and/or computationally implementing models, for example, can demonstrate that accounts are identical or overlap even when their verbal descriptions (i.e., informal specifications) are seemingly divergent. This can be due to, firstly, multiple theories being indeed more similar in essence than previously thought, paving the way for theoretical unification of a seemingly disjoint literature (e.g., Kelly, Mewhort, & West, 2017). Or secondly, theories which are indeed different being less computationally explored and thus less constrained in their current state (e.g., Olsson, Wennerholm, & Lyxzén, 2004). These kinds of discoveries about how we compartmentalise, understand, and predict human capacities are why iterating over, and thus refining, theory, specification, implementation is vital.

Research programmes light on modeling do not have a clear grasp on what is going in the area highlighted in red of Figure 2. These areas of psychology might have many, often informal, theories, but this is not enough (Watts, 2017). Neither is more data — however open, it will never solve the issue of a lack of formal theorising. Data cannot tell a scientific story, that role falls to theory and theory needs formalisation to be evaluated. Thus, while modelers often use the full scale of the path, reaping the benefits of formally testing and continuously improving their theories, those who eschew modeling miss out on fundamental scientific insights. By formalising a research programme, we can search and evaluate in a meticulous way the space of the account proposed, i.e., “theory-guided scientific exploration” (Navarro, 2019, p. 31). As shown using the pizza example, non-modelers remain unaware of pizza problems and may not realise they are implicitly running a different model (in their head) to what they specify.

Discussion

We hope to spark dialogue on the radical role computational modeling can play by forcing open theorising. We also presented a case study in building a basic computational model, providing a useful guide to those who may not have modeled before. Models, especially when formalised and run on a digital computer, can shine a light on when our scientific expectations are violated. To wit, we presented a path function model of science, radically centering computational modeling at the core of psychology. Computational models cannot replace, e.g., data or verbal theories, but the process of creating a computational account is invaluable and informative.

There are three routes that psychology can take, mirroring Newell (1973): *a*) it might bifurcate between research programmes that use modeling and those that do not; *b*) it

might unite in so much as research programmes will contain some modeling to force the creation, refinement, and rejection of theories; and *c*) we carry on by asking questions that are not secured to a sound theoretical mooring via computational modeling. These are not completely mutually exclusive possibilities — some components from each can be seen in the present.

For *a*) bifurcation of the field, theoreticians, scientists who mostly inhabit the red area of Figure 2, will be free to practice modeling, e.g., without having to run frequentist statistics on their models if inappropriate. No constraints will be put on individual scientists to pick a side, e.g., Einstein was active in theoretical and experimental physics. Unlike in the present, it will be easy to publish work containing only modeling at the theory level without direct reference to data (something rare currently, although possible, e.g., Guest & Love, 2017; Martin, 2016, 2020).

In the case of *b*), mass cooperation to work on “larger experimental wholes” (Newell, 1973, p. 24), is perhaps realistic given projects that involve many labs are commonplace (e.g., Botvinik-Nezer et al., 2020; Silberzahn et al., 2018). We advise cautious optimism since these collaborations are operating only at the data and hypothesis levels, which are insufficient to force theory building. Notwithstanding, such efforts might constitute the first step in understanding the logistics of multi-lab projects. On the other hand, modelers often already currently work on a series of related experiments and publish them as single experimental whole (Shiffrin, 2018).

The third possibility, *c*) more of the same, is the most dire: “Maybe we should all simply continue playing our collective game of 20 questions. Maybe all is well [...] and when we arrive in 1992 [...] we will have homed in to the essential structure of the mind.” (Newell, 1973, p. 24) Thus, the future holds more time-wasting and crises. Some scientists will spend time attempting to replicate atheoretical hypotheses. However, asking nature 20 questions without a computational model leads to serious theoretical issues even if results superficially are deemed replicable (e.g., Devereux, Nardin, Baumgaertner, & Buzbas, 2019; Katz et al., 2018).

A way forward

Psychological science can change if we follow Figure 2 and radically update how we view the place of modeling. The first step is introspective: realising that we all do some modeling — we subscribe to frameworks and theories implicitly. Without formalising our assumptions, in the same way we explicitly state the variables in hypothesis testing, we cannot communicate efficiently. Importantly, some have started to demand this shift in our thinking (e.g., Morey et al., 2018; Oberauer & Lewandowsky, 2019; Szollosi et al., 2019; Wills et al., 2017).

The second step is pedagogical: explaining what modeling is and why it is useful. We must teach mentees that mod-

eling is neither extremely complex, nor does it require extra skills over those we already expect they master, e.g., programming, experimental design, literature review, and statistical analyses techniques (e.g., Epstein, 2008; Wills et al., 2017; Wilson & Collins, 2019).

The third step is cooperative: working together as a field to center modeling in our scientific endeavours. Some believe the replication crisis is a measure of the scientific quality of a sub-field, and given that it has affected areas of psychology with less formal modeling, one possibility might be to ask these areas to model explicitly. By extension, modelers can begin to publish more in these areas (e.g., in consumer behaviour, see Hornsby, Evans, Riefer, Prior, & Love, 2019).

In order to ensure experimental results can be replicated and re-observed, we must force theory building; replicability in part depends causally on things higher up the path (also see Oberauer & Lewandowsky, 2019). Data and experiments that cannot be replicated are clearly important issues. However, the same is true for theoretical accounts that cannot be (re)instantiated as code. In the same way that questions such as “should results of preregistered studies count as stronger evidence than results of not preregistered studies?” questions like “should results of computationally modeled studies count as stronger evidence than those of studies with only a statistical model?” must be actively discussed (e.g., Szollosi et al., 2019).

Thus, while it may superficially appear that we are at odds with the emphasis on the bottom few steps in our path model (hypothesis testing and data analysis, recall Figure 2) by those who are investigating replicability, we are comfortable with this emphasis. We believe the proposals set out by some to automate or streamline the last few steps are part of the solution (e.g., Lakens & DeBruine, 2020; Poldrack et al., 2019). Such a division of labor, might help maximise the quality of theories and showcase the contrast — which Meehl (1967) and others have drawn attention to — between substantive theories and the hypotheses they generate. We imagine a “best of all possible” massively collaborative future where scientists allow machines to carry out the least creative steps and thus, set themselves free to focus wholly on computational modeling, theory generation, and explanation.

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