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An epistemological framework for the validation and verification of computational models

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Abstract

Agent-based simulations have become increasingly prominent in various disciplines. This trend is to be appreciated, but it comes with challenges: while there are more and more standards for design, verification, validation, and presentation of the models, the various meta-theoretical strategies of how the models should be related to reality often remain implicit. Differences in the epistemological foundations of models makes it, however, difficult to relate distinct models to each other. This paper suggests an epistemological framework that helps to make explicit how one wishes to generate knowledge about reality by the means of one's model and that helps to relate models to each other. Because the interpretation of a model is strongly connected to the activities of model verification and validation, I embed these two activities into the framework and clarify their respective epistemological roles. Finally, I show how this meta-theoretical framework aligns well with recently proposed framework for model presentation and evaluation.

Keywords: Agent-based modelling, epistemology, models, validation, verification

Introduction

1.1 Agent-based modelling becomes ever more prominent. As many others, I welcome this trend. But with the growth of the field, and its growing interdisciplinary nature, the absence of standards in terms of model presentation and interpretation becomes ever more apparent (Lee et al. 2015; Macal 2016; Schulze et al. 2017). While too strict standards would certainly limit the thrive and creativity of our research community, some standardization is required to ensure that models can be reasonably compared and related to each other (Müller et al. 2014).

1.2 Researchers have responded to the need for standards already in multiple practical ways:

1.3 With regard to the presentation of agent-based models (ABM), in particular the description of their aim and functioning, Grimm et al. (2006) have suggested the ODD protocol, which has been updated in Grimm et al. (2010). The ODD protocol is meant to provide a common format for the description of ABMs and aims to facilitate the mutual relation and replicability of ABMs.[1] Müller et al. (2013) extend the ODD protocol to facilitate the description of agent decision making. Similarly, the MoHuB framework tries to provide "a tool and common language to describe, compare and communicate" formal models of human interaction, particularly in the context of natural resource management (Schlüter et al. 2017). Yet another attempt in this direction is the TRACE framework, which has originally been suggested in Schmolke et al. (2010) and updated by Grimm et al. (2014): it seeks to increase the transparency and comparability of simulation models but focuses on the way the functioning of the model gets analysed and documented. Finally, the systemic design of experiments (DOE) offers an excellent framework for the study of model behavior and the presentation of model results in a transparent and comparable manner (Lorscheid et al. 2011).

1.4 In this paper I will make a different, but complementary suggestion to increase the transparency and comparability of computational models: I will not focus on the presentation of ABM and their functioning, but on the ways models are related to reality and thus meant to create knowledge about the system under investigation (SUI). Models always differ from the system they are meant to represent, and there are different epistemological ways of relating one's model to reality. Making differences between distinct epistemological strategies explicit would contribute a lot to a better comparability among computational models.

1.5 The process of relating one's model two reality is connected to the interpretation of a model and entails two important activities: model *verification* and model *validation*, henceforth VV. A great number of different and most useful verification and validation techniques exist and developing new VV tools is an active and successful area of research (Rand & Rust 2011; Lorscheid et al. 2011; Alden et al. 2013; Lee et al. 2015; ten Broeke et al. 2016; Schulze et al. 2017).

1.6 However, there are no standards with regard to VV on two distinct and equally important levels. On the more practical level, there is no consensus on the 'best' tool for either verification and validation. This is because the complexity, the structure and the purpose of the model at least partly dictate the choice of VV techniques (Sun & M ller 2013; Schulze et al. 2017). There is, however, a lively debate on the adequateness of different tools and innovative new methods are constantly developed in the ABM community (Lee et al. 2015; Schulze et al. 2017; Schlüter et al. 2017).

1.7 On the more theoretical level, there is no consensus on questions such as (1) "Is it necessary to verify and/or validate a model?", (2) "To what extent is the verification and validation of a model even possible?", or (3) "If VV are needed, *what kind of* verification and validation is adequate for the model at hand?" These are epistemological questions and they relate to the deeper problem of how a formal model, an agent-based model in particular, generates knowledge about the real system under investigation. While being more abstract, epistemological questions are by no means less important than the more practical questions raised above. Nevertheless, they usually receive much less attention, which is why they are the main concern of the present paper.

1.8 Discussing the coherence of models and their relation to reality is an important activity for every research community and it is essential that these discussions can be carried out effectively. This gets exacerbated, however, by the fact that different researchers often come with different views on how knowledge can and should be created about the system they investigate. Furthermore, the accepted criteria for what leads to an understanding of or knowledge about the system under investigation can be very different between various scientific communities (Lehtinen & Kuorikoski 2007; Baumgärtner et al. 2008).[2]

1.9 Because of this, scholars also understand and value model verification and validation differently. A common framework of how to align these different perceptions to each other would thus not only facilitate the comparison and relation of ABMs and other formal models, it would also help to structure the discussion about the adequate means for models verification and validation, and to facilitate the dialogue among modellers from different disciplines. This paper aims at supplying such a framework, which may complement applied frameworks such as ODD+D or TRACE.

1.10 To achieve this we will take the following steps: In the next section I introduce a very general epistemological framework of how models are used by researchers to create knowledge about the real world. This helps clarifying the different strategies that can be taken to give models epistemic meaningfulness. Then we will relate model verification and validation to this framework, describe the meta-theoretical relation between verification and validation and discuss whether and when models should be verified and/or validated. In a next step, we identify some immediate practical implications from the epistemological discussion above. Finally, we conclude the paper and summarize the implications for future research.

How models generate knowledge about reality

2.1 This section introduces a general epistemological framework that shows how models can generate knowledge about reality. But before the framework gets introduced in the second subsection, we first discuss why the reference to such frameworks is useful.

Why an epistemological perspective on modelling is useful

2.2 Epistemology is "the study of knowledge and justified belief" (Steup 2016). In this field of philosophy one asks questions such as "What are the necessary and sufficient conditions of knowledge?", "What are the sources of knowledge?" or "How can be generate knowledge about the real world?". Although these questions are obviously very important for applied modelling in both the social and natural sciences, explicit epistemological considerations play a comparatively minor role in applied modelling. This is understandable because epistemology is often very abstract. But sometimes it is important, also for those that are usually concerned with very applied modelling problems, to pause to think about and to clarify the epistemological foundation for their work. As Albert Einstein once put it: "The reciprocal relationship of epistemology and science is of noteworthy kind. They are dependent upon each other. Epistemology without contact with science becomes an empty scheme. Science without epistemology is - insofar as it is thinkable at all - primitive and muddled"(Einstein 1949, p. 683-684). Here I will present a couple of reasons for why epistemological reasoning is important and comment on them one by one:

1. Epistemological arguments are important when choosing and justifying one's modeling framework.
2. Epistemological reasoning is indispensable for relating results from different models to each other.
3. It helps identifying advantages and disadvantages of different modeling frameworks and suggests practical ways for combining them.
4. An epistemological framework clarifies what model validation and verification is about, why it is important, and what we can expect from it.

2.3 If asked why one is approaching a given research question with an agent-based model, the usual answers are of the kind "I want to study the role of the particular interaction structure, and in other modelling framework it is difficult to include this structure explicitly." or "The heterogeneity of the actors can be represented very directly in an ABM, and this is important for my research question!". These answers refer to particular epistemological statements because they formulate some preconditions that are required for a model to be suitable to answer the research question of the modeller. Here, the implicit epistemological claim is that there are certain properties of the system under investigation that must be represented in the model for the model to be useful. Some disciplines, economics in particular, stress other properties of models. (Lehtinen & Kuorikoski 2007; Cartwright 2010; Reiss 2011). When describing the research practice of his fellow economists, Rodrik et al. (2004, p. 133) writes: "Historians and many social scientists prefer nuanced, layered explanations where these factors interact with human choices and many other not-so-simple twists and turns of fate. But economists like parsimony." Here, the realistic-ness of particular assumptions receives less attention, but the clarity and simplicity of a model gets highlighted. A similar point is made by Lehtinen & Kuorikoski (2007) who argue that economists (to a large extent) still adhere to a particular (outdated) kind of explanation similar to the work of Kitcher (1989) who himself build on the covering-law model of Hempel & Oppenheim (1948). According to Kitcher, scientific understanding "consists of the ability to logically derive conclusions with a small set of common argumentation patterns" (Lehtinen & Kuorikoski 2007, p. 324). The "common argumentation patterns" depend on what is accepted in the corresponding research community, and in economics the two main ingredients to this argumentation pattern are individual rationality and optimization, and systemic equilibrium. Simulation models do not have their comparative advantage in this kind of explanation (see below), which is why most economists do not use them.[3] To elucidate such epistemological differences (and to critically assess them from all viewpoints) is essential when we want to engage in interdisciplinary collaboration. This directly links to the second point.

2.4 Consider the following example in which the same system was studied with two different methodologies. There is currently a hot debate among policy makers and economists on the potential welfare and job effects of a free trade and investment agreement between the European Union and the United States. Francois et al. (2013) (and many others) have tackled this question with a *Computable General Equilibrium* (CGE) model, the current standard in economic research practice. The authors conclude that the agreement would lead to generally favourable results. Capaldo (2014) use a conventional macroeconomic model to study the same question but expect job and welfare losses for Europe. Which model is ' better', or, which conclusion should form the basis for the decision making of policy makers? Some might argue that the assumptions of Capaldo (2014) are more adequate than those of Francois et al. (2013). Others might trust more in the CGE model because it relies on economic equilibrium, it is easier and thus more transparent and parsimonious. To trace the different sources for the distinctive policy implications, and to prioritise the models in terms of the knowledge they create, we again need to refer to the epistemological questions posed before and using explicit frameworks greatly facilitate this task.

2.5 The previous argument can be made more general: many instances of models of the same modelling framework, i.e. most agent-based models or most general equilibrium models, share properties such as tractability or flexibility.[4] This point is also highlighted by Raza et al. (2014), who criticizes the reliance of the European Comission on several CGE studies in the spirit of Francois et al. (2013), because all share the same fundamental model structure and are biased in the same direction. Put differently, different modelling framework as such have particular advantages and disadvantages. For example, agent-based economic models are - generally speaking - flexible in their assumptions. General equilibrium models, are - again, generally speaking - very parsimonious and often allow for analytical solutions. If we want to relate the results of the models and relate them to each other, we need to keep this general distinction in mind.

2.6 Researchers in the simulation community are often concerned with the question of adequate methods for model verification and validation. But the question of when and why verification and validation is important, and how this relates to the purpose of modelling, receives less attention. However, to argue why a particular method for model validation is important and means to make a statement on how the link between the model and reality should be assessed. This, as any other argument made in this context, is an epistemological argument.

2.7 In all, there are a number of arguments of why epistemology is important. In contrast to the discussion of the adequate means for model verification, the most important point of epistemological arguments is that they are actually made explicit: using an explicit framework helps comparing models because the way they are meant to explain becomes more explicit, transparent, and, thus, more comparable.

How models create knowledge: an epistemological frameworks

2.8 Building upon the work of Uskali Mäki, I developed an epistemological framework that illustrates the way we learn from models and that helps to structure the discussion on the epistemological foundations of different models. It is built upon Mäkis concept of "*models as isolations and surrogate systems*" (MISS, Mäki (2009a,b)) and it highlights the essential part of modelling: to isolate the important from the unimportant.

2.9 In the MISS approach models are considered to have two fundamental aspects. First, they *represent* the real world. This is necessary because the real world, or any system we want to investigate as such, is too complex to be understood directly. This is not alone a practical argument: there are fundamental physical and computational arguments that show that a direct picture of reality is not feasible. Besides these fundamental arguments, such a direct picture would not even be desirable. As put by Robinson (1979), "[a] model which took account of all the variegation of reality would be of no more use than a map at the scale of one to one" (p. 33). To understand reality, we need to reduce its complexity by abstracting from details, thus building a coarse-grained picture of reality which is called a *surrogate* (Mäki 2009a).[5]

2.10 It is this coarse-grained picture that helps us to understand reality. If we observe the real system under investigation at two successive points of time, its state has changed. The mechanisms driving this change are, however, often unobservable and not directly understandable. Therefore, one studies the model one has built as a representation of reality. If the state of the model is recorded at two points of time, it has changed due to the mechanisms built into the model. But in contrast to the real system under investigation, we built the model ourselves and we (should) know about its structure and its mechanisms. Studying the behaviour of the model (e.g. by altering certain parameters or by implementing different functions) is called model *exploration*. Model exploration is not always straightforward, in particular if the model is more complex. But the ABM community has developed some excellent tools that facilitate model exploration, e.g. the *systematic design of experiments* (Lorscheid et al. 2011). If we can understand something about the real world by the exploration of our model, the model is said to resemble the real world. We will return to the question of how the act of 'understanding reality' can be interpreted below.

2.11 Before, we illustrate the the fundamental idea of the MISS approach in figure 1. First, at time $t = 0$, the modeller builds a surrogate S_0 of reality R_0. This process can be thought of as a mapping g from reality to the model. Because the complexity of the model S_t is necessarily lower than that of reality R_t, we might call the g the *complexity reduction function*.

2.12 The real system is undergoing regular changes, which is why R_t usually differs from R_{t+1}. The mechanisms underlying this change can be thought of as the composite transition function $r : R \to R$. This function is not directly identifiable by the researcher. Therefore the reference to the model is needed. The model also changes over time, according to the transition function $s : S \to S$. This transition function is, however, known, or at least it can be identified via the process of model exploration.

2.13 Looking at the figure suggests two immediate channels through which we can learn something about reality by using our model. One could first compare the model at $t = 1$, i.e. S_1, with reality (R_1). This means to compare the states of the model with that of reality. If we speak about future states of the real word, exploring the model into this direction means to predict the future states of reality. Another option to use the model to conjecture the mechanisms operating in the real world. Note that capturing some of the mechanisms operating in reality may or may not lead to a similarity between R_1 and S_1.

2.14 One may first consider identifying mechanisms or making good predictions is similar, or complementary, but this is not necessarily the case: One may either infer states of the real world correctly without having used adequate mechanisms in the model, or make incorrect predictions even if one has implemented the right mechanisms. Consider, for example, chaotic systems. Here one knows that an exact prediction is impossible precisely

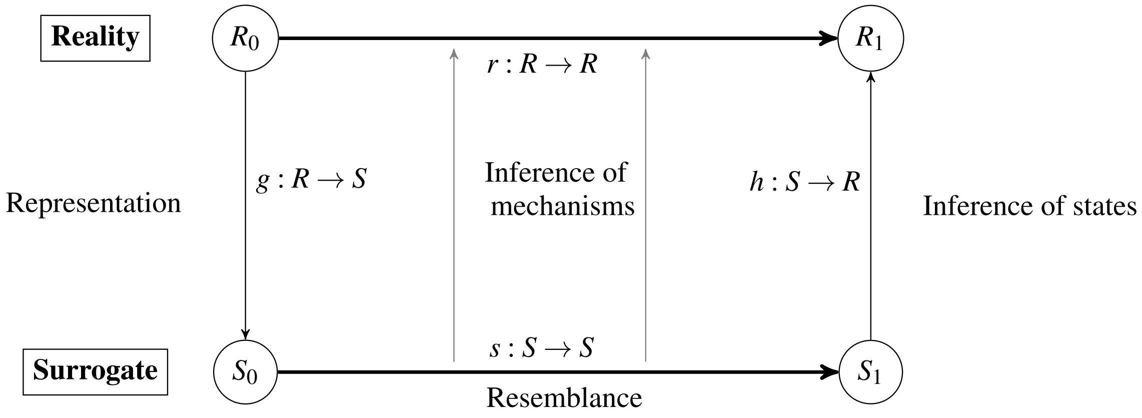


Figure 1: A functional illustration of how the MISS framework clarifies the relationship between models and reality.

because one knows the mechanisms governing the dynamics of the system. A practical example is the evolution of technology. In Arthur (1989), a model of technology choice, it is impossible to predict *ex ante* which technology will be the dominant one (or even if a single technology becomes dominant), but the behaviour of the model is nevertheless very well understood.

Aligning model verification and validation within the epistemological framework

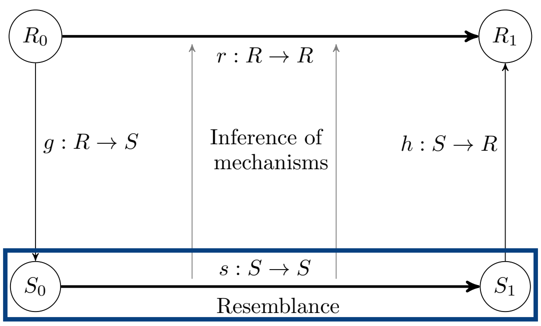
3.1 The epistemological framework developed in the previous section allows us to be precise about the role of verification and validation in the modelling process. While some authors suggested to dismiss the terms because of their ambiguous and careless use in the literature (e.g. Augusiak et al. (2014), or Schulze et al. (2017)), I believe that, precisely defined, they can highlight two important aspects of model evaluation, which are both important, but conceptually distinct. For the sake of transparency of the argument I relate my terminology to that of Augusiak et al. (2014) in the appendix of this paper. There, I also highlight the value-added of the terms 'verification' and 'validation', which I will now clarify.[6]

3.2 With *verification* I mean the testing of whether the model does what it is supposed to be doing, i.e. that it is is free of bugs and other implications not intended by the modeller . This usually involves two steps: (1) study what the model is doing; (2) compare this to what the model should be doing. The first step was referred to as *model exploration* in the previous section. Given this definition, sensitivity analysis would also be considered some form of model verification since it exclusively aims at understanding the behaviour of the model. For more details see e.g. Beck (2002), or Rand & Rust (2011) for a nice summary and ten Broeke et al. (2016) for a review of different tools for sensitivity analysis. The best method for model verification is, of course, a mathematical proof that certain inputs produce a particular output.

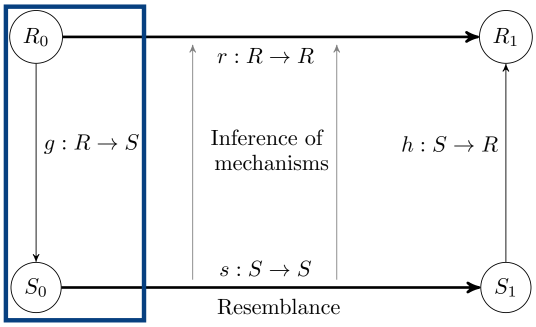
3.3 Model *validation* means to test whether the model is actually a reasonable representation of the system under investigation (Rand & Rust 2011, p. 187). Because 'reasonable' can have different meanings, there are different forms of model validation to be discussed below.

3.4 I will now align model verification and validation within the framework developed above. As indicated in figure 2a, model *verification* is concerned with the internal *consistency* of the model. Examples of methods that are used to verify models are unit testing (i.e. explicit tests for important aspects of the code, e.g. via assertions), code walkthroughs (i.e. an explicit description of what every line of code does), or degeneracy testing (i.e. testing whether the code produces the desired output for extreme values of input).

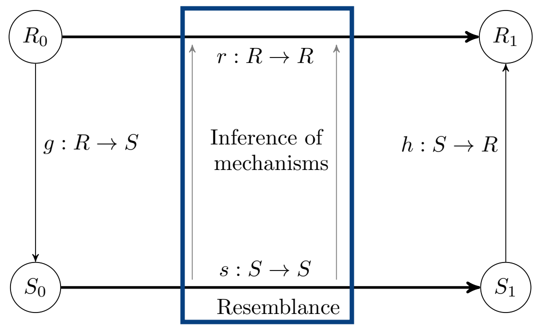
3.5 Considering these methods and keeping in mind that "confirming that the model was correctly programmed was substantially more work than programming the model in the first place" (Axelrod 1997) we might want to keep the effort needed for verification at a minimum and thus ask the question: "What can we do to make model verification easy?" Firstly, we should build *simple* models. The simpler the model, the easier verification (ten Broeke et al. 2016). This is because the simpler the model, the fewer variables and mechanisms one has to



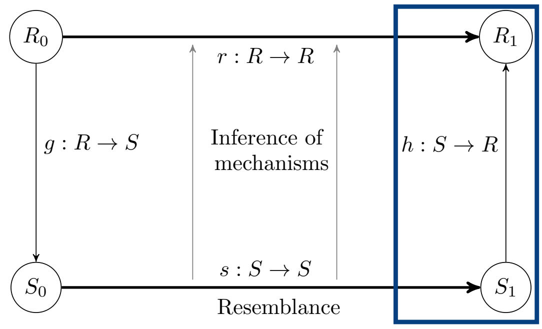
(a) Model verification is concerned with the internal consistency of the model.



(b) Input validation concerns the representation of the SUI in the model.



(c) Process validation asseses the representation of real-world mechanisms within the model.



(d) Output validation addresses the fit of the model or its ability predict future states of the SUI.

Figure 2: The place of model verification and the different forms of validation within our epistemological framework.

check. In the best case, the model is in a form that makes it even amendable for analytical proofs. Secondly, we should build *transparent* models. Tools such as the systematic DOE (Lorscheid et al. 2011) or the various protocols reviewed in the introduction can help to increase model transparency. And the more transparent the model, the easier verification: a model that is written in simplified equations, well-documented computer code or a clear language is - *ceteris paribus* - easier to be verified than other models.

3.6 There is - epistemologically speaking - only one form of model verification (but there are several verification methods). But there are several forms of validation and they partly echo the different perceptions researchers have in mind when they talk about 'understanding reality' (see above). There are (at least) the following four forms of model validation (Tesfatsion 2017):

1. Input validation
2. Process validation
3. Descriptive output validation
4. Predictive output validation

3.7 In contrast to verification, these four activities assess the relation of the model to reality. I will discuss the four forms one by one and relate them in the next subsection. In the appendix I relate this terminology to that of (Augusiak et al. 2014).

3.8 Input validation - as illustrated in figure 2b - assesses the ability of the model at $t = 0$ to represent certain aspects of the system under investigation. In an ABM of a financial market, for example, input validation concerns the question of whether the number of traders is similar in the real market and the ABM, whether their initial wealth distribution is the same, or whether their decision making procedures match. Some inputs to a model are easier to validate than others. Generally, it is always easier to validate aspects of a model that are a *direct* *representation* of real-world objects (Schulze et al. 2017). For example, human beings are boundedly rational and use heuristics, and they do not directly maximize something such as utility (Gigerenzer 2015). So, representing a human beings not as locally constructive and boundedly rational agents, but as utility-maximizers might be a valid and useful modelling approach, but it makes it much more difficult to validate the model in terms of input-validation (Schlüter et al. 2017). Also, input validation gets facilitated if aspects of reality are represented explicitly: If in our model of the financial market, traders explicitly trade directly with each other, the interaction network specifying their interaction structure can be validated against real-world data. This requires the model to be sufficiently complex. If we use indirect representations to keep the model simple, e.g. an *Walrasian auctioneer*[7], input validation becomes more difficult (Balbi & Giupponi 2009).

3.9 Summarizing, input validation gets facilitated by *sufficiently complex* models that avoid as-if representations, and good data.

3.10 Process validation assesses the credibility of the mechanisms in the model with the mechanisms operating in reality (see figure 2c). Process validation gets exacerbated by the fact that in reality, "most mechanisms are concealed, so that they have got to be conjectured" (Bunge 2004, p. 186). Because mechanism are not directly observable, no model will ever be fully process-validated. But there are many reasonable ways to assess the question of whether the implemented mechanism A is more likely or less likely a mechanism in the real world than mechanism B. These include expert and stakeholder validation (or 'participatory validation') (Voinov & Bousquet 2010; Smajgl & Bohensky 2013), process tracing (Steel 2008, ch. 9), or face validation (Klügl 2008).[8]

3.11 It is indeed one of the main epistemological merits of ABM that they are *generative*, i.e. necessarily suggest mechanisms that can - in principle - be tested concerning their plausibility with regard to the system under investigation (Epstein 2007). This gets greatly facilitated by the rise of object-oriented programming, since the distinction between objects and methods in the model facilitates the interpretative relation to real world objects and mechanisms.

3.12 What kind of models are easier accessible for process validation? First, the more direct the representation of the objects and the mechanisms of the real world, the easier the assessment of the mechanism (Macal 2016). Object-oriented models are usually easier to process-validate because objects in the model often correspond to objects in reality, and methods correspond (at least partly) to mechanisms. Second, the model benefits from a modular design.

3.13 Next we turn our attention to *descriptive output validation*. Here we ask to what extent the output of the model can replicate existing data (see figure 2d). Or, to speak with figure 1, we compare the states S_i with R_i for all $i > 0$. For example, if we have built a model for the UK economy, we may compare the time series for GDP from the model with real-world data on the GDP of the UK.

3.14 Although descriptive output validation is maybe the most commonly used form of validation (at least in economics), there are some problems with this kind of validation that we have to keep in mind:

1. Empirical risk minimization: in most cases, one is interested to minimize the prediction risk of models. Because the empirical risk of a model is unobservable, one often uses the empirical risk as an approximation or estimator for prediction risk. This is a mistake because the empirical risk gets minimized by choosing a model with many free parameters, while prediction risk increases with too many free parameters.
2. Overfitting: this is a direct corollary from the first point. If a model has so many free parameters that it can very well be calibrated to existing data, it is very likely that it performs poorly for new data.
3. Equifinality: usually, we can think of many mechanisms that can bring about the same result: the mechanism-to-function mapping is many-to-one (Gräbner & Kapeller 2015, p. 435). Therefore, the calibration of a model to existing time series alone tells us relatively little about what mechanisms were actually at work.

3.15 A good illustration of the limits of descriptive output validation is given by Janssen (2009) who discusses the famous Anasazi model and shows how many important questions still remains open, despite the model having a very nice fit to the historical data. Without additional validation forms being applied (in this case particularly further process validation), the model can 'explain' the dynamics of the Anasazi only in a limited way.

3.16 What makes a model easy to validate in terms of descriptive output validation? *Ceteris paribus*, the more complex the model and the more free parameter it has, the more successful it will be in terms of descriptive output validation. Grimm (2005) describe the practice of 'pattern oriented modelling' as a less naive form of descriptive output validation: here, one tests how several model specifications can replicate an observed patter, eliminates the unsuccessful one and proceeds with more detailed patterns until all but a very few candidate models remain.

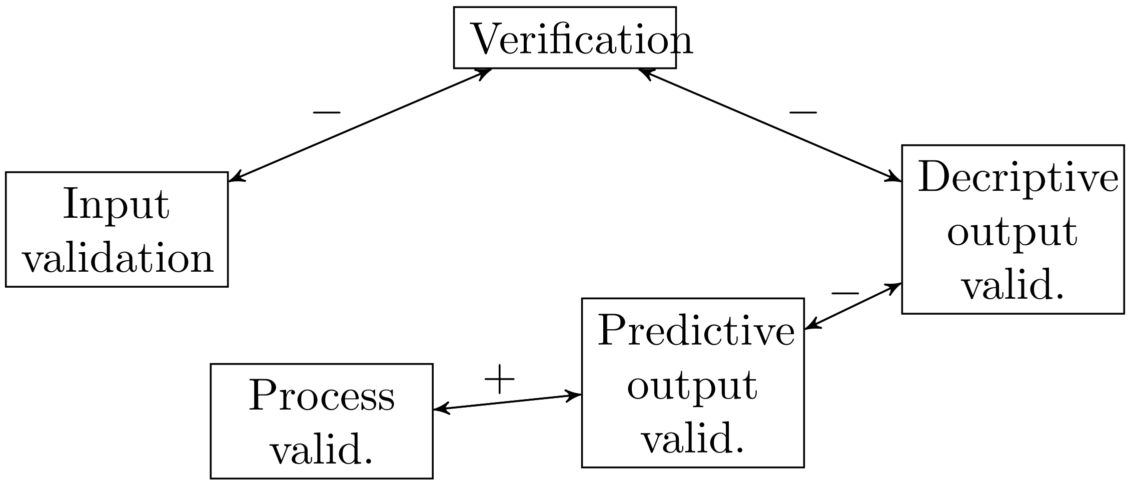


Figure 3: The relationship between verification and the different kinds of validation.

3.17 Finally, *predictive output validation* basically asks how well the model can be trained to predict future states of the system. Its idea is also illustrated in figure 2d, but in contrast to descriptive output validation, the real world data gets separated into a training set and a test set. This way, one effectively addresses the problem of over-fitting and empirical risk minimization. This form of model validation is extremely illuminating, but not always applicable because of data requirements. Furthermore, it should be aligned with process validation, since being able predict without knowing why one is able to predict is often not sufficient to understand the system under investigation.

The trade off

3.18 What is the relation between verification and the various types of validation? Is there a model design that scores optimal in all four activities? Unfortunately, for the single model this is not the case. As illustrated in figure 3, there are trade-offs in terms of model design: making a model easily amendable to one kind of verification/validation makes it more cumbersome to validate/verify for another kind.

3.19 We first consider the relationship between input validation and verification. Here, researchers often face a trade-off because a successful input validation gets facilitated by a direct and detailed representation of the system under investigation, but verification gets easier if the model is more parsimonious. Also, the ease of verification due to model simplicity often comes at the expense of generality, since it is not clear to what extent the model applies to situations for which the (strict) assumptions are not applicable (Cartwright 2007).

3.20 When turning to the relationship between verification and descriptive output validation, we again observe a tension in terms of model design: descriptive output validation produces the best results for models with many degrees of freedom, while verification is easiest for simple and parsimonious models. As in the case of verification and input validation, there is a trade-off between a more complex and better validated, and a simpler, better verified model.

3.21 The next relationship to be considered is that between descriptive and predictive output validation. It is very clear that there is a trade-off involved because the relationship between the two kinds of validation mimics the well-known trade-off between risk-minimization and empirical risk-minimization in inferential statistics: the more degrees of freedom we give to our model, the easier it is to calibrate it to the data we have, but the greater the risk for over-fitting.

3.22 Finally, we turn to the relationship between predictive output validation and process validation, which seems to be complementary. There are a couple of reasons for why I consider this relationship to be complementary: Firstly, one argument in favour of representing real-world mechanisms explicitly in formal models is that such models are easier to generalize, both in terms of time and space. Since training a model could be considered to generalize theory from small data sets, models that explain in terms of mechanism should also be useful for prediction. Secondly, training a model works through letting the algorithms explore patterns in the data,

Aim	Verification	Input valid.	Process valid.	Descript. valid.	Predict. valid
Provide predictions	★	★			★★★
Explain what happened	★★★	★★	★★	★★★	
Scenario analysis	★★★	★	★★		★★

Table 1: A possible prioritization of verification and the different types of validation, depending on the model purpose.

and these patterns are likely to be caused by real-world mechanisms.[9] Therefore, a model that performs well in resembling mechanisms of the SUI should at least not perform worse in predicting the system's future behaviour as a model that does not capture these mechanism well. Finally, real-world mechanisms are usually unobservable. And while the techniques of process validation mentioned above are certainly effective, process validation should always be complemented by other validation techniques. Predictive output validation, if feasible, certainly seems to be an excellent choice from a practical perspective.

Validation and the purpose of a model

3.23 Considering these intricate relationships and trade-off's between various forms of validation and verification we must ask whether some there can be a reasonable prioritization among them. If this were true, one should design a model such that it maximizes its performance in terms of this form of verification/validation and then turn to the other one by one, depending on their respective importance. Unfortunately, such a general ranking is not feasible. Rather, what kind of VV is needed depends on the *purpose* of a model (Suarez et al. 2010, p. 136).

3.24 Table 1 suggests an assessment for the various forms of VV for three typical model purposes. There are many more purposes for modeling one could think of (see e.g. Epstein (2008)), and the ranking suggested here can surely be debated. The key message of the ranking is, however, that, depending on the purpose of the model, decisions among competing designs must be made and the decision in favour of one design might entail a better performance in one kind of VV at the cost of a comparatively worse performance in another kind of VV.

3.25 There is no general rule for a concrete prioritization and the respective kind of VV but the comparison among different models and their interpretation can nevertheless be facilitated if the design choices are made as transparent as possible and are explicitly justified and related to the purpose of the model. Here, my proposal aligns well with existing frameworks for model presentation according to which the model purpose should be made very explicit (e.g. Grimm et al. (2014)).

3.26 While the claim that validation should follow the purpose of the model is widely accepted, there are important exceptions: As argued by Lehtinen & Kuorikoski (2007), different disciplines have different conceptions of what counts as 'understanding'. Based on these conceptions, they may not follow this claim. Economists, for example, prefer parsimonious models that can be solved analytically within the *maximization-cum-equilibrium approach*. This constraints the set of admissible modelling methodologies and validation techniques, and thus there is a bias towards particular forms of VV in economics (in particular towards descriptive output validation).[10] Using explicit epistemological frameworks such as the one suggested here, may facilitate to identify and to overcome such biases via interdisciplinary discussion and reflection.

Some immediate practical implications

4.1 Two immediate practical implications for applied modelling design follow from what has been claimed in the previous sections: Firstly, there are some design principles that are at least never harmful, but frequently useful when assessing the relation between a model and reality. These are principles such as a *modular modelling design* and the strive for *transparency and clarity* in the exposition of the model. Secondly, while it may not be possible to design a model that performs very well in terms of all kinds of VV, one can sometimes combine the respective strengths and weaknesses of *several* models via the practice of *sequential modelling*.

4.2 Sequential modelling refers to the practice of starting with a very simple and stylized model and then building more and more complex models that are all verified by aligning them (in the sense of Axtell et al. (1996)) with the previous, simpler model. In the best case, the first, and thus simplest, model is amendable to analytical proofs. Usually, such simple models are purely equation-based. One can then proceed by building an agent-based model that can be aligned with this simplest model. This way, one can "transfer" some of the rigour of the simpler model to the more complex model. If successful, this practice allows one to appreciate the advantages of simple models in terms of verification also for the more complex models, which have their strengths in model validation.

4.3 Take the investigation of Henderson & Isaac (2017), two economists studying agrarian production, as a simple example: The authors start with a general-equilibrium model of agrarian production that allows for an analytical solution. The model, however, represents poorly the structure of modern agrarian production. To preserve the rigour of the original mode, Henderson and Isaac develop an agent-based model that replicates the functioning of the original model. Thanks to its modular structure, the agent-based model can then be extended to include some essential features of modern agrarian production that are beyond the scope of the original model. In the end, the authors have a model that is a good representation of the reality the authors are interested in, but that is also well verified because of its sequential construction.

4.4 Unfortunately, the practice of sequential modelling is not always applicable: the system under investigation must be such that a very stylized model can at least remotely related to this system. This may not always be the case. Also, when relating the increasingly complex models to each other, one faces the problem of when one model simulates another. This has been discussed more extensively in Axtell et al. (1996) under the topic of 'Aligning Simulation Models' and subsequent work. Despite its potential difficulties, however, there are already a couple of examples where the practice of sequential modelling has been very successful, see e.g. Axtell et al. (1996), Bednar & Page (2007), Gintis (2007), or Henderson & Isaac (2017).

Conclusion and outlook

5.1 In this paper I have introduced an epistemological framework that illustrates the various ways models can help us to understand reality. We have argued that using such frameworks is useful because they help to exemplify the different epistemological foundations of various models. This way, we can more transparently justify the modeling framework we have chosen, compare the results of different models and choose more rationally between modeling frameworks.

5.2 The framework was also used to distinguish and illustrate various forms of model validation and verification. This distinction is meaningful, because not all models are directly related to reality, but they can nevertheless be useful and should be verified. We have seen that there are different ways to relate a model to reality (i.e. to validate it) and that there are trade-offs with respect to model design: some designs facilitate VV in one sense, but make it more difficult in another. Which kind of VV should receive priority depends on the model purpose, but there are some design principles that are always useful and never harmful (e.g. a modular design).

5.3 Based on these considerations I have argued that different modelling approaches have different comparative advantages and disadvantages with respect to VV: agent-based models, for example, seem to have a comparative advantage in terms of input validation and process validation. A comparative disadvantage of agent-based models is model verification: while a great number of excellent verification methods exist, ABMs usually do not allow for the most successful verification technique: a mathematical proof.

5.4 Based on this observation I suggested the practice of sequential modelling. Similar to the idea of sequential modelling is that of using a pluralism of models.

5.5 Finally, I want to build on our epistemological elaborations to answer two questions mentioned in the beginning: (1) "Is verification and validation necessary?" and (2) "Is verification and validation possible?". With regard to the first question: There might be instances of where we are only interested in predicting future states of the system under investigation and where model verification plays a minor role. But aside from this I cannot think of any instance where model verification is not important. There are many reasons for why we should know how our models work, which is why every model in this world should be properly verified.

5.6 Validation becomes important as soon as we want to use our model to make informed statements about the real world (e.g. Schulze et al. (2017)). This is not always the case: Gerard Debreu, a mathematician by training and one of the most influential economists of the previous century claimed that "theory has a mathematical form that is completely separated from its economic content." (Debreu 1986, p. 1265) and that with every new interpretation the model gets another meaning. The consequence for the model builder is that she does not need to care for any relation of her model to the real world. This can then be done by people that "apply" these models. I believe that this strategy is not very successful in the social sciences, engineering and the natural sciences, but more useful in mathematics (see Augusiak et al. (2014, p. 123-124) for a similar claim). But there are some cases in which models do not need to be validated at all, especially in the case of 'proof-of-concept' models that illustrate an idea and that may later serve as building blocks for more complex models. But as soon as we want to use our model to make informed statements about the real world, validation becomes important, and the kind of validation we should seek depends on the particular kind of statement about the world we want to make.

5.7 So, verification is always and validation often important. What about the feasibility of VV? If we consider our framework as illustrated in figure 2, verification is concerned only with the internal structure of a model. At least for simple mathematical models a nearly complete verification is often feasible. Verbal models can never be verified with certainty, and computational models reside somehow in the middle. So, while *complete* verification is possible only for a small subset of models, *sufficient* verification is a feasible and attractive desideratum.

5.8 Considering validation, the situation becomes more complex. Firstly, some forms of validation are easier (e.g. descriptive output validation) while others (e.g. process validation) are more difficult. Secondly, a complete validation will always remain impossible, even if one focuses on one particular form of validation (e.g. input validation). We simply cannot perceive reality in its entirety such that we could compare the model to this complete description of the real world. Even in the century of big data (in which still many data problems prevail (Schulze et al. 2017)), there will never be the perfectly validated model.

5.9 But the fact that *complete* verification and validation might be impossible does not release us from the duty to strive for the best verification and validation that is possible and adequate for our modelling purpose, and to be transparent regarding how we want our models to relate to reality and on how we have assessed this. Frameworks such as the one presented here hopefully complement existing frameworks of model presentation and evaluation to facilitate this task.

Appendix A: Relating the framework with the 'evaludation' framework of Augusiak et al.

Augusiak et al. (2014) argue that the terms 'validation' and 'verification' should be eradicated because they are ambiguously and barely mean anything any more. Instead they propose the general term 'evaludation'. I believe that - properly defined - the terms 'verification' and 'validation' are useful and highlight the difference of studying a model itself or the relation of a model with reality. The term 'evaludation' blurs this distinction for the sake of generality. Nevertheless, I think the framework and the terminology of Augusiak et al. (2014) is extremely useful for model analysis, particularly because it is well adjusted to the natural modelling cycle. But I believe it would be useful to complement it by an explicit, epistemological framework as presented in this paper.

To facilitate this task, table 2 relates the terminologies from my framework to that of Augusiak et al. (2014).

There are three aspects of the relationship worth mentioning: Firstly, Augusiak et al. (2014) do not mention all forms of validation that are possible. I believe that what they term "Model output corroboration" might be interpreted more broadly to capture also descriptive output validation and process validations.

Secondly, Augusiak et al. (2014) advocate a model building process that contains some aspects of the sequential modelling approach: they assume one first builds a conceptual, non-computational model, that is then computerized. The aligning of the final and conceptual model is therefore rightfully considered an important step in the modelling cycle. In my framework, this is not necessary the case. I agree that it is good practice to have a conceptual model that gets then computerized, but since both the conceptual and the final model can be both verified and validated (the former at least conceptually), I think that even here the distinction between verification and validation (together with the idea of sequential modelling) makes sense.

Thirdly, the framework is by no means incompatible with my epistemological framework. This is not surprising, because both frameworks have different, but complementary aims. From a pragmatic viewpoint, it seems to me that if both frameworks are used jointly, every step in evaluadation procedure should explicitly distinguish between activities concerned with the model, and activities assessing the link of the model with reality, and be explicit about how the latter could be established. In figure 4 I suggest a way to accommodate explicit epistemological considerations into the evaluadation framework (thereby slightly altering the terminology of Augusiak et al. (2014)), but other ways to relate the framework are certainly possible.

Term from Augusiak et al.	Reference to VV terms	Comment on the relationship
Data evaluation	NA	This step is rightfully highlighted by Augusiak et al. (2014) as an essential step within the modeling cycle, but it does not need to be part of an epistemological framework.
Conceptual model evaluation	Verification / Input validation	Augusiak et al. (2014, p. 125) consider this as the “assessment of the simplifying assumptions underlying a model’s design [...] including an assessment of whether the structure, [...] form a logically consistent model.” This step has elements of model verification (e.g. the test of all assumptions are logically consistent), and validation (e.g. the assessment of the assumptions capture the essence of the real system).
Implementation verification	Verification	Augusiak et al. (2014, p. 125) use this step to ensure that the modelling formalism is accurate and that the computational model does what it is supposed to do. This corresponds to verification in the sense I use the term.
Model output verification	Input validation	Augusiak et al. (2014, p. 125) define the aim of this step as “to ensure that the individuals and populations represented in the model respond to habitat features and environmental conditions in a sufficiently similar way as their real counterparts.” This step involves some aspects of verification, but mostly corresponds to input validation.
Model analysis	Verification	Here, Augusiak et al. (2014) are concerned with testing the sensitivity of the model to changes in the model parameters, and the understanding of how the model results have emerged. This step is clearly about verifying the model since no link to reality is investigated.
Model output corroboration	Predictive output validation	In their final evaludation step, Augusiak et al. (2014, p. 125) seek to compare “model predictions with independent data and patterns that were not used, and preferably not even known, while the model was developed, parameterised, and verified.” This is basically the definition of predictive output validation.

Table 2: A clarification of the relationship between the terms used byAugusiak et al. (2014) and my epistemological framework.

Notes

[1]It’s use has been encouraged by prominent outlays, including JASSS. However, it is more prominent in some disciplines (e.g. ecology), and less frequently used in others (e.g. economics). This illustrates the difficulty of introducing commonly accepted standards into a lively research community.

[2]For an excellent illustration of the consequences of different conceptions of understanding see Lehtinen & Kuorikoski (2007) who study the reluctance of economists to use agent-based simulation models.

[3]As for Lehtinen & Kuorikoski (2007), it is important for me to stress that these descriptions of the economic way of theorizing are descriptive, and do not mean that I endorse this kind of theorizing. I believe taking it seriously reminds us to value rigour and parsimony, and to question whether the complexity of a model is adequate, but in general Kitcher’s epistemology is not desirable in a normative sense.

[4]General equilibrium models are a standard modelling approach in economics. One specifies few representative agents that maximize their utility and imposes and equilibrium restriction on the complete system. The classical introduction is given in Mas-Colell et al. (1995).

[5]This is why both philosophers and cognitive scientists often refer to the notion of ‘cognitive representations’ and ‘mental models’. As famously put by Forrester (1971, p.):“Every person in his private life and in his business life instinctively uses models for decision making. The mental image of the world around you which you carry

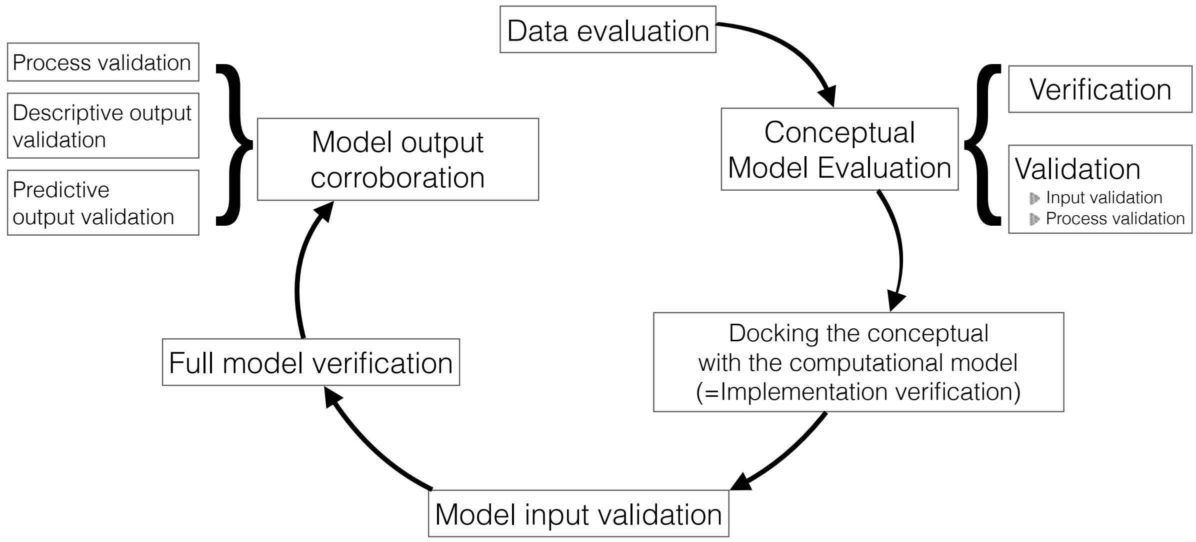


Figure 4: One possiblity to include epistemological considerations into the evaluadation framework. Where necessary one should explicitly refer to the framework outlined in figure 1.

in your head is a model. One does not have a city or a government or a country in his head. He has only selected concepts, and relationships between them, and uses those to represent the real system."

[6]See Reiss (2011, p. 251) for a similar distinction made from a more philosophical perspective. He compares the epistemology of simulations to that of experiments and argues - rightfully, I believe - that they are the same. For an experiment you also have to check first whether the data created tells you enough about the functioning of your model/experiment, and then whether the model relates well to the real system you want to investigate.

[7]The Walrasian auctioneer is a fictitious entity that is used to tell a story about how simple general equilibrium models reach the equilibrium: every buyer and seller communicates a price to the auctioneer and no trade takes place before this fictitious entity announces the set of prices for which there would be an equilibrium between supply and demand. As one might have expected, the decision problem for this fictitious entity is very hard (Axtell 2005).

[8]While process validation is an obviously tedious task, the merits of models that explain via the provision of mechanism gets more and more acknowledged and the validation of models in terms of mechanisms becomes more and more a *desideratum* (Steel 2004; Deaton 2010; Reiss 2011).

[9]Under a mechanism, we understand a sequence of states, or a pathway within a concrete system (Bunge 2004; Gräbner 2017).

[10]This claim gets nicely illustrated by the unwillingness of some economists to test their rational expectation models via rigorous statistical test but rather prefer to calibrate them, simple because "these tests were rejecting too many good models" (Thomas Sargent in Evans & Honkapohja (2005)).

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