Will AI Make Simulation Superfluous? - A Subjective Stocktaking –

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Abstract. Based on current success stories using AI methods, this paper examines the relationship between the problem-solving methods AI and system simulation. An analysis of the process steps of the two approaches highlights the fundamental difference between the black-box approach of learning methods and the glass-box approach of structure-explaining simulation models. The mutual benefits of the two approaches can then be explained using four use cases. A further result of the analysis is the question of the extent to which simulation and AI methods can lead to the same or different results. To this end, the concept for a structural analysis is presented, which is based on the idea of analysing the intersection between the results of AI and the simulation method.

AI in Competition with Classic Simulation Methods ?

Forecasts on the development of demand and the content of engineering professions show, on the one hand, that human intelligence will probably continue to be irreplaceable, especially for creative tasks, but on the other hand, around 50 per cent of working time could be replaced or at least significantly supported by artificial intelligence methods. ([1],[2],[3],[4]).

These forecasts will be analysed in more detail here with regard to the method of dynamic system simulation. In this area, too, there are initial approaches to generating simulation models automatically or at least with AI support, although the limits of AI are still evident at present [5].

On the other hand, there are many examples of applications in which the use of AI and classic simulation have been successfully combined. We will look at these examples in detail in the section on possible use cases.

However, in order to be able to work out the mutual advantages, we will first compare the way the simulation method works with the general approach of data-driven machine learning (ML) (as a sub-area of AI). The potential efficiency gains of combining the methods will then be presented in more detail. Following these fields of application of coupling and/or combining AI and simulation, which are already established in practice, an approach will be presented at the end that uses experiments on a structural, set-theoretical basis to determine whether the two approaches actually (only) produce the same results or whether they (can) find qualitatively different solutions.

1 Analysing the Process Steps oft the Isolated Methods

1.1 Simulation Method

The aim of using the simulation method is always to develop a model in a formalism that enables the algorithmic processing of time progress within the scope of a simulation run. The trajectories of the model variables over time derived from the model description allow statements to be made about the modelled system within the previously agreed validity range of the model. The decisive step in this procedure is the establishment of the formalism or the rules according to which the temporal dynamics of the modelled system unfold. (Figure 1).

There are two different approaches: In the general case, experiments must be carried out on the real system and their results then analysed for dependencies and rules using human intelligence alone.

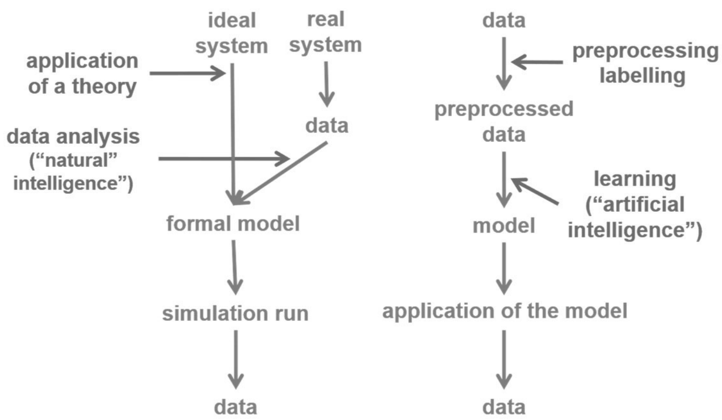

Figure 1: Comparison of the work steps between modelling and data-driven learning processes.

The totality of these rules represents the formal model, which can then be further processed algorithmically - usually in a simulation environment. If there is already prior knowledge about the system to be modelled in that a general theory (e.g. conservation of energy, network theory, etc.) can be used, no explicit system experiments are necessary.

Instead, the laws of the theory are applied, from which the formal model can be derived. In both cases, however, the end result is a set of rules that can be used to transform the input data (consisting of initial state and parameter assignment) into a set of output data (results of the simulation run). If this approach is viewed in the form of an input-output box, this box is transparent and the modelled system is represented by an explanatory structural model in the glass box.

1.2 Machine Learning Method

In contrast to the simulation method, many AI learning methods work with a black-box approach: the essential starting point for this is system data that has already been collected. This data must first be carefully pre-processed. Pre-processing usually involves homogenisation and - in the case of supervised learning methods - classification (labelling) of the input according to the expected, correct system response. This classification of the input data sets using human intelligence introduces system knowledge into the process so that a model can then be developed in an automated learning phase without further intervention. In the work phase (model application), this model responds to any input with an output that - again only within the agreed validity range - corresponds to the learnt classification.

1.3 Comparison of Approaches

A significant difference in the resulting model lies in the already explained black-box view of the learning methods on the one hand and the glass-box view of the explanatory simulation models on the other. Accordingly, the learning methods require a statement about the corresponding correct output for each individual input, but no information about the causal relationships. How the output is derived from the respective input does not have to be introduced as rule knowledge. Accordingly, when interpreting the results of learning models, the question of why cannot be systematically clarified because iso-morphic relationships are not necessarily formed between the system and the model that replicate the causal chain of the system.

Another difference lies in the amount of system data required: Not only must the learning data contain all possible classes of result data, it must also be available in such large numbers that the statistical approaches used in automatic learning can assume a sufficiently large population. In contrast, the rules of the glass-box model can also be found or derived from a small amount of data, even without any system data at all when using the theory approach.

However, uncertainties often arise when setting up the rule set for simulation models, which an algorithmic model specification does not allow due to the requirement of unambiguousness. In these cases, the introduction of randomised parameters that obey defined distributions helps. However, this approach practically always and necessarily entails a complex statistical treatment of the simulation results. Thus, the savings in terms of the amount of input or learning data are relativised in the end by a higher effort on the output side, because the results of a simulation run alone are not meaningful and must be statistically validated by a large number of simulation runs in the sense of a random experiment.

With these general considerations in mind, constructive synergies between the two different approaches will now be presented in the form of five use cases.

2 Combined AI and Simulation Methods: Use-Cases

The use cases described below highlight approaches to the combined use of AI methods and simulation that have actually been realised and are not just available in the form of research results or pilot studies.

For this purpose, a Google search was carried out on the web using the search terms "AI and Simulation".

The pages listed here deal directly and intensively with this topic:

- Simplan [6]
- Siemens "Simultelligence" [7]
- Anylogic [8]
- Mathworks [9]
- Fraunhofer IISB Erlangen [10]
- Merkle CAE Solutions GmbH [11]

Although each of these providers has a slightly different focus, there are strong similarities and overlaps that can be summarised in the typical use cases presented here. Although one source did not contribute directly to the development of the use cases, it should be noted here as an aside: If a coupling of AI and simulation succeeds conceptually and in terms of software technology, the LRZ Munich points out that the fundamentally different hardware concepts required for efficient calculation must then also be combined and optimised. [12]

2.1 Using ChatBot for Knowledge Engineering and System Analysis

The first use case supports a process step in the development of simulation models that was not explicitly mentioned in the description in Section 1, but nevertheless constitutes an important part of the work on the way to a correct, complete and consistent model: system analysis and knowledge engineering, which is often carried out in the form of interviews with experts from the target domain of the model to be developed during the analysis phase. These tie up the time of experts with system knowledge. Many questions relating to model development could be clarified with the help of a chatbot that accesses the existing database of the application domain.

It will certainly not be possible to answer all questions, but such an application should significantly reduce the time other-wise required for expert interviews. On the research side, a similar approach was investigated by Freydenlund et al [5].

2.2 Analysing Online Sensor Data using Pre-trained Learning Models

A second use case is the coupling of an AI-based, pretrained model with online sensor data under real-time conditions. However, this naturally requires the AI model to have been trained with all potential states of the system beforehand.

In addition, the question arises as to whether simply recognising the irregularity is sufficient or whether the system's set of rules must also be transparent in order to take countermeasures.

2.3 Generating Learning Data for AI using Simulation Models

It is often problematic to obtain consistent learning data for the learning phase of the AI. Such data could be generated artificially through classic simulation. The advantage: it is structured, classified and can be generated in any quantity, subject to computing time. However, the double modelling effort is immediately apparent: both a simulation model and an AI model are used.

Glass-box system understanding must be available in order to be able to generate learning data in a meaningful way. The real-time speed of the AI approach therefore comes at the cost of considerable additional effort in the design phase. In addition, the problem of "rare events" becomes relevant: Even if these have been explicitly generated as learning data through prior simulation, it must be ensured that they are correctly recognised and learned as such by the AI and not ignored as outliers.

2.4 Testing the AI Model in a Virtual Simulation Environment

Conversely, a simulation model can be used to test the AI model: The AI model is coupled with a digital twin in the form of a simulation model of the target environment and so its subsequent use in the real system can be safely tested in this virtual environment. Again two models, the simulation model and the AI model must be developed for this scenario.

A similar scenario arises when AI-supported simulation models are coupled uni- or bidirectionally with IoT sensors, drones or other physical entities. [13] This coupling enables the continuous adaptation of the simulation state to the real system state.

2.5 'Hybrid' Simulation Models

The last use case deals with the situation where the system knowledge in a complex, modular-hierarchical model is not sufficient to describe the behaviour of individual components based on rules. If the interface is known, these components could be replaced by an AI model previously trained on a black box basis.

In this case, no causal relationships need to be specified at this point of detail, although the interpretation of the results of the overall model becomes more complicated with this type of model design because the causal chain is interrupted by the affected model component.

3 Are the Approaches Equivalent in Terms of their Results?

As the sources cited in each case show, the use cases presented in Section 2 are state of the art and can be pragmatically adapted to the task and evaluated in terms of costs and benefits. However, the question arises as to whether there is further potential that is not yet covered by these use cases. One point of reference is the frequently described experience that automatic data analysis reveals system relationships that were previously unknown.

With this in mind, one might ask whether the results obtained from classical simulation on the one hand and those generated by AI approaches on the other are or can be equivalent. Or is it conceivable that AI-based methods produce results that could not be achieved through classical simulation? The same applies, of course, in the opposite direction: are there results from the simulation approach that cannot be explored using AI methods?

The following setup is intended to provide an outlook on future research activities. A complex, possibly adaptive input-output system is given, which is modelled once by a rule-based simulation model and alternatively by an AI/ML model.

If we now consider the quantity of results that the two approaches deliver, three different cases arise in the general case: The sets of results of the approaches completely overlap (a), they are disjoint (b), or there is the case of a true intersection (c). It can be assumed that cases b) and c) are more realistic, as both approaches are already used in practice and at least comparable results are obtained. However, the question then arises whether complete equivalence (case c) can actually be observed, or whether there are system states that only become visible when one of the both approaches is used.

The authors' subjective and preliminary recommendation is therefore to "think together" simulation and AI. This combined exploration of the state space of a complex system promises interesting and possibly new insights into the dynamics of the system modelled.

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