Can (and should) Automated Surrogate Modelling be used for Simulation Assistance?

Veronika Kurchyna[1,2], Jan Ole Berndt[1], and Ingo J. Timm[1]

[1] German Research Center for Artificial Intelligence (DFKI)
Smart Data & Knowledge Services, Cognitive Social Simulation
[2] Corresponding Author: veronika.kurchyna@dfki.de

Abstract. Recent advances in machine learning may be leveraged by researchers in the context of agent-based modelling. With the help of surrogate models, machine learned models based on samples of a more complex agent-based model, computationally expensive evaluation methods such as sensitivity analysis and calibration may be supported and sped up. To explore the outlook on using surrogate modelling to assist simulation, possible criteria for eligibility are defined. With regards to a use case such as simulation-based crisis management and decision support, existing literature in different fields is reviewed to assess the current state of the art and potentials for holistic approaches to surrogate modelling-based simulation assistance. This work acknowledges the potentials of surrogate modelling in combination with automated machine learning, but finds no evidence that the current state of the art allows for an accessible, wide-spread usage.

Keywords: Agent-based Modelling · AutoML · Surrogate Modelling · Metamodelling · Simulation

1 Introduction

Science and development are often expressed as a workflow – a series of steps that researchers need to complete in order to deliver a methodologically sound scientific contribution. In some instances, workflows are facilitated by tools, while for others only loose guidelines exist. Simulation is one of the many fields in which researchers typically work in established workflows which are often only conceptually described, such as the often-cited simulation process defined by A. Law[1]. We examine the case of Agent-Based modelling (ABM) and how methods of artificial intelligence and machine learning (ML) may be used to support researchers in their workflows towards high model quality.

Simulation using ABMS is a way of examining existing systems for various purposes, such as prediction, optimisation or other questions of study[2]. However, such simulations can easily become computationally expensive. Scientifically important tasks, such as sensitivity analyses and calibration, are time-consuming. With recent advances in machine learning, surrogate modelling is viable approach to facilitate computationally expensive tasks: with a machine-learned surrogate model, the execution of the actual model is simulated in a fraction of the required time[3]. However, as different literature reviews have shown in the past, the use of a surrogate model is rarely a choice of methodological design but a research point in itself: while there exists ample evidence for the potentials of metamodelling for ABMs, there is a lack of studies in which the usage of a surrogate model was a design choice to answer other research questions. Researchers who wish to benefit from the advantages of surrogate models have access to different guides, yet no tools or frameworks that facilitate the task of transforming an existing ABM into a surrogate model that can be used for further study. Difficulties may be added by the choice of simulation framework and connection to other frameworks and scripts which handle analyses.

Ideally, researchers would be able to easily create a surrogate model of their complex micro-scale model and perform different analyses to verify their models before proceeding with experiments. Therefore, this paper aims at exploring the state of the art regarding surrogate modelling for sensitivity analysis and calibration of agent-based models, as well as existing advances towards the usage of automated machine learning (AutoML) and other contributions towards tools and methodological improvements of surrogate modelling in the context of agent-based modelling. Finally, based on the examined literature, the viability of widespread usage of machine learning-based simulation assistance is discussed.

2 Foundations

Simulation and Agent-Based modelling: When the observation of a real system is not possible, simulation is a means of gaining insights using an artificial recreation of the system[4]. Such simulation models may show various degrees of complexity. With large numbers of parameters for configurable simulations, researchers encounter the curse of dimensionality: the parameter space is opaque and difficult to analyse due to the exploding number of configurations[5].

One approach to simulation is agent-based modelling. Individual components of a system are represented as autonomous entities. These agents form large-scale patterns based on small-scale decision-making mechanisms. This effect is commonly referred to as 'emergence' and is a major characteristic of ABMs, showcasing that a system is often more than the sum of its individual parts[6]. Different architectures and formalisations have been proposed to unify the concepts, implementations and description of ABMs. While they are capable of recreating complex systems, ABMs are also computationally expensive[6]: large models may contain thousands of individual agents that compute, process, interact and impact the simulated environment. As such, the previously mentioned problem of exploding parameter space is exacerbated in agent-based models.

Verification and Validation of ABMs: Verification assesses whether an implementation fits the formal and theoretical specification – a verified model is (largely) bug free, implements the selected algorithms correctly[7]. Validation examines whether the implemented model actually represents the real system[7]. While the validation of assumptions and concepts prior to implementation is meant to reduce the risk of implementing an inaccurate model, pilot runs may still reveal that inaccuracies remain, requiring a restart of the design process. One possible reason why validation may fail is the inability of the system to create expected behaviours or observations from the real world. While some techniques, such as validation by experts who can comment on the plausibility of results, are only loosely structured at best, other approaches to verification and validation are highly formalised and allow for possible automation[8].

Sensitivity analysis and calibration are two techniques of particular interest. Sensitivity analysis measures the impact of parameters on model behaviour – this process allows identifying redundancy or parameters whose behaviour deviates from the conceptual design – such as important parameters having too little an impact on model behaviour or larger influences than intended by the model design. As such, a good sensitivity analysis allows for better exploration of the behaviour of the model[9]. While sensitivity analysis only conducts experiments to learn more about the model behaviour, calibration can be used to find parameter settings that produce desired outcomes. This is a necessary step that must be made before experiments – models need a baseline parameter configuration that represents 'normal' or default behaviour before researchers can examine how the variation of parameters further impacts the model's behaviour. Both methods are computationally expensive with growing parameter spaces. As such, it may be beneficial to find a way to cut down on computation time.

Surrogate modelling: One way to use machine learning in the context of ABMs is the learning of surrogate models, also referred to as metamodels. These models 'simulate' the actual simulation, predicting the output for a given input parameter combination[3]. The original model is sampled using a space-filling method such as hypercube or Sobol designs[10]. Different techniques, such as artificial neural networks, can be used to represent the ABM in a compact form. It is important to note that while surrogate modeling/metamodelling often refers to models of another model obtained by machine learning, the idea of simulating more complex models predates the recent popularity of machine learning, using statistical and mathematical methods instead[13]. Thus, the terms generally refer to all types of models that emulate a more complex model and are used interchangeably in this work. Generally, though, the metamodels in question will be models obtained by some type of machine learning approach.

While basic approaches surrogate the entire model, other approaches choose composite, hierarchical concepts which may only surrogate parts of the model. The resulting model can be used for further analyses. By doing so, the execution time is cut drastically[3] – however, this comes at an obvious expense: a large number of samples will be required to learn a model of sufficient accuracy[10]. The use of a surrogate model only makes sense when less samples are needed than when calibrating a model or performing a sensitivity analysis.

There are several different approaches to creating surrogate models of ABMs. Besides obvious design decisions, such as the choice of learning algorithms, researchers also need to handle a more fundamental question: what is being surrogated? While some models may choose to create the entirety of the model as a single blackbox machine learning construct, others may choose a hierarchical approach in which only parts of the model are replaced with surrogates – be it agent groups, individual agents or other components of the model which may cause bottlenecking and thus could profit from substitution through a surrogate. Designs that work closely with the model and substitute parts of it for usage in other components cannot be used for finished models that were not conceived with such usage in mind. As such, we are interested in methods for the emulation of entire models for maximized reusability of findings.

Automated Machine Learning: The issue of sample numbers is exacerbated when concepts such as AutoML are involved. In this field, researchers aim to automate different aspects of machine learning. Hutter et al. compiled the state of the art in AutoML, which is recommended lecture for readers who wish a deeper insight into this field[11]. The range of possible aspects that may be automated using AutoML includes hyperparameter tuning for a given algorithm or the selection of validation methods. The goal of AutoML is granting accessibility to domain users with no machine learning background – a strong AutoML pipeline would work with a given dataset and find the best combination of processing steps, algorithms and hyperparameters to enable researchers to employ machine learning in their work. Obviously, beyond research, AutoML is also a topic field in private companies, though the application in commercial context is not further considered here. Still, the relevance of this field means that researchers in the discipline of ABM may profit from the current boom in AutoML applications, both commercial and open source, to leverage recent developments in an ABM context.

3 Motivation - When Does Automation Make Sense?

Given the effort that is required to build a surrogate model, one has to ask: when does it make sense to build it at all and when is the added work on using AutoML to achieve this goal justified? The use case for such a simulation workflow assistance tool could be a simulation which fulfills the following criteria:

1. The Model is expected to be calibrated more than once. The amount of time saved through metamodelling grows with each reuse of a learned model.
2. The Model and its inputs are expected to change periodically. Embedding recurrent relearning in an automated process optimizes the overall workflow.
3. The Model is expected to be used by people without technical expertise. Humans without expertise may not recognize when a model needs to be recalibrated or relearned and when a workflow pipeline needs to be adjusted.

One possible use case which fulfills such criteria is simulation-based crisis management and decision support. When working with changing data, such as new infections during the Covid-19 pandemic, re-calibration is necessary. Once calibration is a step that is executed regularly, the time saved using a surrogate model might exceed the implementation efforts. Further, when more fundamental aspects of the model change, such as complex inputs like population structure and disease characteristics, detection of changes and automated re-learning of an old model provide valuable support for the maintenance of systems which integrate simulation models as a continuous service[12], rather than a one-time simulation study. Finally, when used by human domain experts such as decision makers and stakeholders of such support systems, automated workflows can conceal the underlying complexity of model maintenance and thus bridge the gap between ABMs and users who wish to include them in their work.

4 Overview of related works and state of the art

This section provides a brief overview of important questions, such as the availability of toolkits for ABM, existing applications of surrogate modelling for agent-based models, evidence of feasibility and applications for analysis. Additionally, topics regarding AutoML and methodology will be considered, examining contributions that raise further questions. This work presents an overview of important examples of relevant works that showcase the use cases and open questions in surrogate modelling for ABMs. Publications were chosen based on accessibility, recency, relevance to the key topics of this paper.

Surrogate modelling for ABMs:

Several studies have explored the intersection of agent-based models (ABMs) and machine learning. Before proceeding to surrogate modelling using methods of machine learning, the work by Fadikar et al.[13] is particularly mentionable. The researchers demonstrated that machine learning is not the only way to benefit from the advantages of surrogate modelling. A moderately complex ABM for the simulation of an epidemic was used to display the potential of quantile-based emulation, a mathematical method which does not rely on machine learning methods to handle the complexity of behaviour space and multivariate outputs. These findings are important, given that the choice of surrogate method impacts the performance of the resulting system. Still, given the recent advances in machine learning since the publication of [13] it is worth exploring newer insights into the combination of ABM and machine learning without discarding the potentials of more classical approaches.

Amaral et al.[14] conducted a comprehensive review on metamodelling for simulations. Their investigation confirmed the growing interest in the optimisation as usecase for surrogate models. However, only 3% of the works examined were agent-based models. Instead, most metamodels act as surrogate for numerical and discrete event type simulations. Dahlke et al.[15] examined existing literature regarding the combination of ABMs and methods of machine learning and found that an overwhelming majority of research focuses on integrating machine leaning to enhance the learning capabilities of agents. Their literature review only found a small number of publications in which surrogate modelling was used to analyse the output and system dynamics of ABMs. As such, using surrogate models for this purpose is not a widely explored field yet. Both publications confirm the same point: Only a small subset of publications that employ machine learning in an agent-based context do so for the purpose of metamodelling. At the same time, out of the publications that employ metamodelling for the analysis of simulation models, only a small fraction of the examined models is actually agent-based.

That small intersection was explored by Pietsch et al.[16]. Their examinations approach the question of surrogate modelling from a practical perspective by examining different techniques, the quality of the results and the implementation effort. The study found that most approaches have good accessibility in terms of available guides and explanations. It was found that especially Bayesian Emulators and Machine Learning were suitable for the calibration of ABMs via metamodels. Both methods also perform well in sensitivity analyses as well as output prediction. While the authors found detailed guides for different approaches, the findings did not include any tools that reduce human involvement in the usage of metamodelling. More importantly, their literature review did not extend to questions of automatisation, assistance or the trade-offs between traditional model analysis and surrogate modeling-based approaches.

As a result, there is a need for a closer inspection of different aspects relating to the possibility of a semi-automated toolkit for model analysis using surrogate modelling, combining different areas of research and analysing the state of the art from different perspectives.

In Summary, the combination of ABMs and surrogate modelling is in its infancy compared to other types of simulation, though growing interest is observed.

Feasibility of Surrogates for ABM Many studies focus on feasibility – this includes speed increase, model quality and the accuracy of results. Angione et al.[17] compare the usage of nine different methods for the emulation of an ABM with different sample sizes. Using a moderately complex model with 22 parameters, they found that artificial neuronal networks perform well on large sample data sets that portray the complexity of the parameter space. Edali and Yucel[18] examine a supply chain model with potentially complex behaviours and how potentially chaotic outputs may be handled by metamodels. The authors conducted experiments with different sampling techniques and ML methods to compare the approaches in terms of performance and predictive quality. Similar to other studies, good performance was found, though all methods were imperfect in their result predictions even on a small model, raising questions regarding the suitability of metamodelling for large, complex ABMs.

De Leeuw et al [19] apply two different methods of surrogate modelling to an ABM for airport terminal operations. In this case, the methods are not only applied to experimental models for the sake of metainformation about the surrogate model method, but to a model that is in research use, which aligns with the primary research interest of this literature review. In this study, a Random Forest approach and an Artificial Neural Network have been used and compared in terms of learning and execution speed as well as result quality. No significant differences were found, with ANN only slightly outperforming Random Forests on some metrics. In terms of result quality, this study largely confirms that metamodels typically deliver adequate approximations of the original model[17]. Similarly, Yousefi & Yousefi[20] demonstrate the use of metamodels for the analysis and calibration of complex ABMs based on real world data through the examination of human resource planning in emergency departments. As the researchers point out, ABMs have valuable potential applications in decision support when used for forecasting based on real world data, further underlining the potentials of integrating metamodels into ABMs actively used for decision support.

Besides the examination of the feasibility and quality of metamodelling, researchers also identify potentials to improve the methodological quality of surrogate modelling as part of a scientific workflow. Gore et al.[21] focus on ways to improve the quality of metamodels in terms of transparency and input complexity by providing predicates that express the relationship between variables. Additionally, Bosse[22] investigated another issue that is persistent both in the domain of ABMs and machine learning: inaccurate inputs for models based on real world data. This issue is exacerbated in any system in which there is a continuous flow of data and simulation. The author presents a hybrid approach that leverages the benefits of different technologies to minimize the negative impact of varying input data quality. An important factor in this approach lies in the hierarchical composition of model components. Further, given the scale of the model, this approach is situated within the context of models which may benefit from the usage of surrogates. Such works provide helpful guidelines for researchers who may want to design models with the usage of surrogate modelling in mind.

In summary, while the usage of surrogate models is feasible, the integration of ML may not necessarily provide significant benefits over other approaches. Further, the volume of necessary training data may cancel out the speed increase during deployment. The lack of examinations on large models raises the question on what types of models can be surrogated effectively at all.

Analysing ABMs using surrogate models Besides the feasibility of implementing a surrogate model, many publications examine whether the quality of results obtained from a learned surrogate live up to the promised potential of this approach. As such, publications of this category do not question the accuracy of predicting simulation models, but specifically focus on the usage of these metamodels for the purpose of model analysis.

Lamperti et al.[23] examine how surrogates can be used to explore the parameter space of an ABM and how a learned model can be used for efficient calibration. In this publication, the authors highlight an important issue in the creation of surrogate models: *how are outcomes to be labelled and what sort of behaviour is desired and intended?* The proposed solution is to require at least one viable parameter configuration which has to be provided by the users. Thus, this work highlights a potential approach in which calibration, parameter space exploration and model training are parts of an interlinked workflow.

Zhang et al.[24] also applied a machine learning algorithm to learn a surrogate to facilitate the calibration of agent based models with low knowledge of the parameter space and a limited amount of sampling. The paper draws a positive conclusion, seeing potential in this approach to circumventing issues with the calibration of models with large and complex parameter spaces.

Besides the calibration of ABMs, the analysis of the sensitivity of different parameters is an important step towards understanding the dynamics of the system.

While many publications focus on model calibration, only few works examine the parameter space. Bargigli et al.[25] demonstrated that the analyses facilitated by metamodelling are an important contribution towards the exploration of ABMs and the complex interactions between different model components across the parameter space. While no machine learning methods were used, their work still provides further proof of the usefulness of metamodelling. However, like many ABMs discussed in the context of technique and methodology, only a small, primarily mathematical model, was employed to illustrate the effectiveness of the chosen approach. Ten Broeke et al.[26] made similar observations in their analysis of surrogate models and their usefulness in analysing agent-based models. The authors defined a workflow which takes an important characteristic into account: an ABM may have different distinct behavioural types depending on parameter combinations. As such, their proposed approach includes the identification of such behaviour types, allowing finer sensitivity analysis on parameters that create certain patterns.

All presented papers share the same conclusion: surrogate modelling is a viable approach to facilitate the exploration of complex ABMs. However, research often drifts into different directions and halts at open questions, ranging from questions of performance, to ease of integration, to specialisation of analysis methods enabled by the usage of surrogate models. As such, the authors see high potential in surrogate modelling for ABMs with branching opportunities for further research and valuable ideas and insights on the improvement of the scientific value researchers can obtain from the usage of metamodels.

In Summary, surrogate modelling can be used for the study of ABMs in the form of sensitivity analyses or calibration. The variety of open questions raised in different publications hints at a need for further study before wide-spread usage.

AutoML and Human Experts: To anticipate changes in the original model that require retraining of the surrogate model, automated machine learning for the optimal learning methods may be an interesting approach. In such a case, automated machine learning would be used to learn optimal techniques to re-learning the surrogate model based on changes in the original model. Of course, such a use case would require there to be significant benefits of automated machine learning compared to human expertise or non-interference, not only for automated machine learning in general, but this specific use case as well.

Zöller and Huber[27] present an extensive examination of automated machine learning frameworks in an in-depth manner, highlighting several issues currently encountered by users in this field. By comparing several open source AutoML frameworks against baseline strategies on a high volume of real world data, the researchers provide not only a theoretical AutoML approach, but also examine existing solutions. The experiments concluded a low variation of performance between the different frameworks and approaches. Most importantly, the different automated pipelines did not outperform random search, leading to questions regarding the outcomes of both this study as well as alternative studies contradicting these findings.

Vaccaro et al.[28] examined the variety of problems for which machine learning may be helpful and the different requirements for solutions offered by a generalized machine learning pipeline through a systematic literature review. The authors also provide a proof of concept for workflow representation, starting at data processing. Unfortunately, as it the case with many of such works, the utilised data and models are not publicly accessible and readily available for use by other researchers interested in applying this concept to their own work. In the same year, Xin et al.[29] approached the usage of AutoML from a practical perspective by conducting interviews with individuals who use AutoML tools in their work. These interviews, despite the small sample size, provided insights into the perceived benefits and disadvantages of existing AutoML frameworks and may act as a guideline for the design of frameworks with similar goals.

These publications show that AutoML will likely gain further interest in the coming years, with new advances opening the accessibility of machine learning for different purposes. As such, there is potential for the usage of AutoML for the learning of surrogate models. However, given mixed results in terms of quality, it is likely that the field of AutoML may require further advances, before an out-of-the-box usage of any framework is preferable over manual implementation when only one use case with little to no future changes is to be automated.

In summary, while highly anticipated in the research community, AutoML is currently not at a stage where human expertise can be replaced effectively.

Toolkits for ABM: Finally, we need to take a look at toolkits, frameworks and programs that provide simulation assistance for an existing simulation model by facilitating or automating tasks. While literature reviews generally focus on recent works, we also consider older contributions given the lack of recent developments. It is unlikely that there exists a single tool that covers the vast spectrum of different simulation frameworks. As such, it is important to note which framework and language a tool was developed for.

Lorig[30] examined theoretical frameworks, specifications and existing toolkits for various domains in simulation studies and analysed the possibility for assistance and automation of conducting simulation studies based on hypotheses as a central concept of goal-oriented simulation. During the assessment of existing tools and frameworks, a lack of multi-purpose tools for the automation of common tasks was confirmed, with most works relying on outdated versions of frameworks. The original author's systematic literature review observes that while there exist strong theoretical concepts and foundations for simulation assistance, actual implementations are rare and typically poorly maintained.

This conclusion is supported both by the works of Cariklar et al. [31], who detailed a framework meant to facilitate the testing and validating of models implemented in Repast Simphony as well as Garcia and Patón[32]. They also present a contribution towards the analysis of Repast models with the help of the RRepast package, which provides tools and functions to integrate repast simulations in an R script. Further, Perumal and van Zyl[33] presented a framework for the parametrization of agent-based models using surrogate models. The researchers analyse the performance of different sampling- and surrogate model methods which can be exchanged within their presented framework. However, like many such projects, the paper lacks information on implementation languages and open source disclosure of the model and the proposed framework beyond the concept. As such, while this is a further display of the feasibility of such a project, accessibility remains an issue. While the toolkit developed by [31] was not available for public download at the time of writing, the RRepast package is still available. However, this package highlights another issue with older works: even if the framework is still available for download and compatible with newer language versions, they do not leverage newer techniques and concepts which have been introduced after publication.

However, Stonedahl[34] demonstrated a successful toolkit via a major contribution for the NetLogo framework. BehaviourSearch represented an advance in the calibration and exploration of ABMs through the examination of genetic algorithms, faciliatedt by providing a graphical user interface. Similarly, NetLOGO also offers the possibility to automate experiments using a factorial design, though external tools are necessary to perform analyses on resulting output data. Through close cooperation with framework developers, toolkits can become part of the default package and integrate seamlessly into the ecosystem of the framework, avoiding issues of maintenance and compatibility in the future.

Given the rapid development of technology, especially with advances in ML, it is worth revisiting the idea of such toolkits from an updated, modernized perspective. [34] is an important example of a toolkit done right, proving that despite challenges, this accessible type of simulation assistance is possible.

In summary, two major issues persist in the domain of toolkits for ABMs: incompatibility with other technologies and poor maintenance, if available at all.

5 Conclusion

The efficient analysis and calibration of agent-based simulation models remains an open issue. This work examined the use of surrogate modelling to address issues of efficiency. Further, through the inclusion of AutoML, a workflow for actively used models with changing data and model properties can be built. Simulation-assisted crisis management is a possible use case in which such an approach may be advantageous. Sighting of the relevant literature on the current state of the art has shown that there exists ample proof of the feasibility of such a system: the learning of surrogate models and their usage for the analysis and calibration of ABMs at a decent quality is possible. However, while research indicates potential in this field of study, the authors identified a series of problems related to different aspects of a comprehensive, ML-supported solution to the ongoing issues regarding model analysis.

Studies confirm that large volumes of sample data are needed to learn a reliable surrogate model, which means a large number of model executions is necessary. At the same time, analyses, experiments and calibrations also require large numbers of model runs which could be performed instead. Therefore, questions regarding the sense of such substitutions are valid. The issue is further exacerbated by the fact that current AutoML approaches do not outperform randomness or manual tuning. Therefore, the inclusion of AutoML into a pipeline designed to compensate for model changes currently offers no significant benefits.

Finally, ABMs regularly used by untrained users with constantly shifting input parameters and model characteristics may be common for some areas of ABM research, but does not take the needs of other fields into consideration. As a result, the authors judge that other approaches should be examined instead of relying on machine learning. While the methods and techniques discussed in the different papers are fascinating, there is no strong evidence that this technology is ready for wide-spread use in the ABM community.

As future work, the authors intend to examine alternative approaches towards assisted model analysis and calibration. At the same time, periodic checking of the state of the art in ABM conjoined with machine learning is recommended, since there exists potential in this combination of techniques.

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