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PVactVal: A Validation Approach for Agent-based Modeling of Residential Photovoltaic Adoption

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***Abstract*—Agent-based simulation models are an important tool to study the effectiveness of policy interventions on the uptake of residential photovoltaic systems by households, a cornerstone of sustainable energy system transition. In order for these models to be trustworthy, they require rigorous validation.**

However, the canonical approach of validating emulation models through calibration with parameters that minimize the difference of model results and reference data fails when the model is subject to many stochastic influences. The residential photovoltaic diffusion model PVact features numerous stochastic influences that prevent straightforward optimization-driven calibration.

From the analysis of the results of a case-study on the cities Dresden and Leipzig (Germany) based on three error metrics (mean average error, root mean square error and cumulative average error), this research identifies a parameter range where stochastic fluctuations exceed differences between results of different parameterization and a minimization-based calibration approach fails.

Based on this observation, an approach is developed that aggregates model behavior across multiple simulation runs and parameter combinations to compare results between scenarios representing different future developments or policy interventions of interest.

***Index Terms*—Agent-based Modeling; Computer Model Validation; Computer Model Calibration; Innovation Diffusion; Rooftop Photovoltaic Diffusion.**

I. Introduction

A. Motivation

The adoption of rooftop photovoltaic systems by decentral residential actors is commonly seen as a cornerstone of a transformation towards a decarbonized energy system [1]. Yet, the uptake of residential photovoltaic systems fails to meet the needs for achieving ambitious climate protection goals. This is due to numerous reasons, which are not all fully understood (e.g, [2], [3]). Simulation-based models can help to investigate grounds for this shortcoming, as well as analyze policy instruments to encourage a larger uptake of residential photovoltaic systems. For this, agent-based models are seen as an appropriate tool.

While agent-based innovation diffusion simulation models can help to understand both the individual and collective household behavior, as well as the effect of policy interventions on the modeled systems [4], they need to correspond well to the modeled context. In order for simulation-based models to allow inferring the effectiveness of policy measures, modelers need to ensure that the model corresponds 'as closely as possible' to the modeled domain. For this, thorough model validation is crucial. Model calibration, understood as finding a set of input values that allow the model to match the observed data as closely as possible [5], is an important part of model validation.

B. Object of investigation & Research Problem

This article presents the validation framework developed for the PVact simulation model[1]. PVact is an agent-based innovation diffusion model for the adoption of rooftop photovoltaic systems (PV) by residential households developed at Leipzig University. It aims at modeling the decision behavior of individual households embedded in a social and spatial context under socio-economic and attitude-based considerations.

Operational validation (i.e., the comparison of model results and real-world data) of agent-based emulation models is commonly done through model calibration in order to set free parameters of the model before comparing the respective simulation results with reference data [7]. However, model calibration through history matching can be challenging in contexts involving stochastic influences. The remainder of this paper thus investigates issues that can be encountered during the calibration of empirically grounded agent-based technology diffusion models. In addition, it presents a joint calibration-validation approach that is designed to address calibration issues associated with the underlying stochastic nature of these processes. As an illustrative example, the calibration of the agent-based diffusion model for decentral PV systems *PVact* is considered.

C. Structure

This research problem is addressed by describing the calibration of the model through history matching, the discussion of the results and its issues, followed by the development of an approach to evaluate the simulation of different policy instruments of interest to the modeled system. After the model is briefly sketched below, section II presents the framework in which the validation takes place and briefly outlines how aspects of validation other than operational validation were addressed. It emphasizes on operational validation and describes the approach taken in subsequent sections. It thus provides the methodological background for the rest of the article.

[1]As a model instance of the IRPact modeling framework [6], which is published under a GPL-3.0 license under https://github.com/IRPsim/IRPact.

Section III presents the results of the calibration attempt and discusses issues with the followed approach, which leads to the development of a more refined approach coined PVactVal presented in section IV. The paper closes with an outlook to research avenues addressed in future papers (see section V).

D. Summary of the model

PVact is an agent-based residential rooftop photovoltaic diffusion model based on the theory of innovation diffusion [8], the theory of planned behavior [9] and the value-belief-norm theory [10]. Agents represent spatially explicit households based on their socio-demographic and psycho-social identity, as well as their physical living situation. The model focuses on the decision to adopt rooftop-PV systems through a step-based decision process and household-specific utility of the technology. Agents evaluate the technology based on its expected financial performance, their innovativeness and environmental concern, as well as social and local pressure. This is done through a weighted partial utility function that is triggered once agents develop sufficient interest and the technology is feasible for their living situation. Interest is generated through communication with other agents in their social network on a point-basis until a set threshold is reached.

The model contains numerous stochastic dynamics: agents are associated with agent groups, which exhibit different socioeconomic and psychological profiles[2], as well as geographical variation[3]. These groups are described through probability distributions for each agent variable of the model, and during simulation instantiation values are drawn for each agent from these distributions. Similarly, the social network is instantiated randomly with a set number of ties for each agent according to their milieu, with the probability to form a link with an agent from a given agent group based on the affinity between these milieus. For inter-agent communication, communication events are drawn randomly, with conversation partners being any agent with an established link to the agent. During communication, attitudes of agents are adjusted according to the relative agreement algorithm presented in [11]. Finally, agents have a chance to change their living situation (proportional to the rate of construction and renovation associated with the case study).

II. Methodology

Model validation is central to the credibility of models and the use of simulation results. [12] distinguishes between three forms of validation: the theoretical (or conceptual) verification used to assess the adequacy of the *conceptualization* of the real world, external (or operational) validation used to test whether the *simulation results* correspond to the observed data and cross-model validation used to assess in how far the *results of two models* map. To these, [7] adds the forms of internal validation used to determine the correctness of the *software code*, data validation used for assessing *data accuracy and adequacy* and security validation for ensuring minimal *model tampering* through model reconfiguration.

Data validation of the model was ensured through careful selection from different data sources and data processing. Through hosting the model in a modern model infrastructure with an experienced partner, security validation was given. Internal validation was achieved through following clean code-driven software development practices and code testing. Additionally, a toy-model concept was implemented to improve internal validation. Using a series of model configurations exhibiting clear and drastic model behavior further contributed to the conceptual validation of the model. In addition to the toy-model concept, PVact was grounded in existing literature [2], [3], as well as extensive empirical work during model development [13]. Finally, cross-model validation could not be performed as no reference models exist.

A. Operational Validation of PVact

While other forms of model validation can be addressed during model construction, operational validation is only possible once an implementation is finished. Operational (or external) validation is understood as proving the correspondence of simulation results and observed data, i.e. comparison of model results with real time-series. This is usually done through presenting a model instance that reproduces data for a given case study. Often, this is done through calibrating the model with a single parameter set that yields minimal error in a similar model setting.

In a first step, this research addressed this through two case studies describing the adoption of residential photovoltaic systems in a residential context. One such case-study (PV adoption within the city of Leipzig between 2000 and 2019) was used to assess operational validity of the model, whereas another case-study (PV adoption within the city of Dresden between 2000 and 2019) was used for calibration of the remaining free parameters.

Model calibration involved setting the free parameters for the interest threshold (a weighted number of events with exposure to PV for the agents) and the adoption threshold (the minimal utility that a PV system has to be rated at in order to be adopted). Parameters were aimed to be set through comparing simulation results based on different parameter choice with the observed installation of residential PV systems within the city of Dresden based on different error metrics as discussed in section III.

For the case studies, data on installed PV systems by non-commercial entities within the case-study[4], socio-economic Sinus® milieus and purchase power data[5], georeferenced

[2]These are largely based on Sinus® milieus; see https://www.sinus-institut.de/en for further information.

[3]Through zip-codes and the possible buildings associated with them.

[4]taken from https://www.marktstammdatenregister.de/MaStR on a yearly basis per post code.

[5]acquired from MB Micromarketing with address-specific granularity for Leipzig, and street sectional granularity for Dresden.

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building data[6] and construction and renovation data[7] was collected. The street sectional Sinus® milieu and purchase power data was transposed to the address level in Microsoft Excel, using the provided street section identifiers for each address. Georeferenced building data sources were merged in Q-GIS, and then matched with the Sinus® milieu and purchase power data via the address, resulting in a dataset with 49,657 full entries for Dresden, and 48,112 for Leipzig. The data sources and the coverage are shown in table I (for the calibration study) and II (for the validation study).

Table I
DATA SOURCES AND THEIR OVERLAP (ABSOLUTE AND RELATIVE) OF THE DATA USED FOR THE CASE STUDY DRESDEN

Data source	Size	Overlap	
		Absolute	Relative
LoD2[6]	141,772	141,772	100%
Inspire[6]	72,428	51,395	36%
Microm[5]	68,294	49,657	35%

Table II
DATA SOURCES AND THEIR OVERLAP (ABSOLUTE AND RELATIVE) OF THE DATA USED FOR THE CASE STUDY LEIPZIG

Data Source	Size	Overlap	
		Absolute	Relative
Gebäudelayer[6]	145,786	145,786	100%
Inspire[6]	70,979	60,197	41%
LoD2[6]	515,513	53,367	37%
Flurstücke[6]	110,822	50,096	34%
Microm[5]	69,504	48,112	33%

III. RESULTS & DISCUSSION

For the parameter selection required for the calibration of the model, the parameter landscape was analyzed through an iteratively refined grid. In each iteration, a parameter region around the minimal error in the grid of the previous runs was analyzed with increasingly higher resolution. For the analysis, three error metrics were used: the mean average error MAE measuring the average yearly difference of installed PV systems between the simulation data x_i and observed data $\hat{x_i}$ over N years (see equation 1), the root mean square error $RMSE$ as the root of the square of these errors (see equation 2) and the cumulative adoption error CAE as the average error of installed systems between the simulation and real data (see equation 3). To keep computational tractibility, the three error metrics were analyzed in a reduced setting of 1341 agents, while keeping socio-economic and geographical distributions proportional.

$$MAE = \frac{1}{N}\sum_{i=1}^{N}|x_i - \tilde{x_i}| \tag{1}$$

$$RMSE = \frac{1}{N}\sqrt{\sum_{i=1}^{N}(x_i - \tilde{x_i})^2} \tag{2}$$

$$CAE = \frac{1}{N}\sum_{i=1}^{N}\left|\sum_{j=1}^{i}x_j - \sum_{j=1}^{i}\tilde{x_j}\right| \tag{3}$$

The results of the simulation presented in figure 1 show that low parameter values lead to large errors in all used metrics. The corresponding graphs show the error (vertical axis with redder shades corresponding to higher errors and greener shades corresponding to lower errors) over parameter combinations of the interest threshold and the adoption threshold in the horizontal plane.

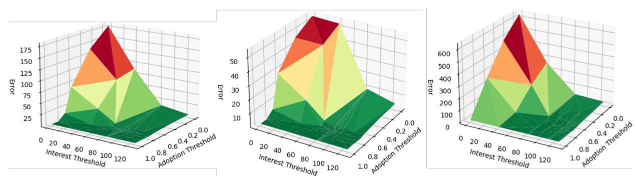

Figure 1. Error between the reference data and simulation results according to the error metrics MAE, RMSE and CAE as described through the equations above.

For other parameter regions, the picture is less clear; A closer look at the error landscape with smaller errors shows large variation of errors between similar parameter combinations that are not consistent throughout the observed error metrics, as seen in figure 2. In this, the variation between different parameter combinations in the horizontal plane is much smaller than in other parameter regions. As the parameter values between low error values (downward facing green spikes) correspond to (relatively) larger errors, the deviations between the corresponding simulation runs and reference data were larger. While there could be very specific combinations that yield larger deviations between the model and the observed data, this high and specific sensitivity seems rather unlikely.

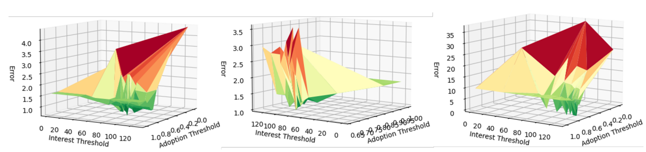

Figure 2. Error between the reference data and simulation results below an error value of 4.5 (MAE), 3.6 (RMSE) and 37.2 (CAE).

Reruns of parameter combinations yielding a small error term furthermore show large deviations in measured error between runs of same parameterization of up to one order of magnitude

[6]with address-specific granularity taken from the INfrastructure for SPatial InfoRmation in Europe (Inspire), and open geodata from the state of Saxony (3D-building layer with the level of detail 2 (LoD2)) for both case studies; additional address-specific data on buildings (Gebäudelayer) and land parcel-specific data on owner situation (Flurstücke) was provided by the city of Leipzig for Leipzig.

[7]taken from https://www-genesis.destatis.de/genesis/online on a yearly basis for Saxony.

for sufficiently small errors in the reduced setting, showing the influence of random model mechanics for well-performing runs. An example of this is seen in figure 3, which shows the PV adoption patterns of the same parameterization (adoption threshold AT of 0.7092 and an interest threshold IT of 114).

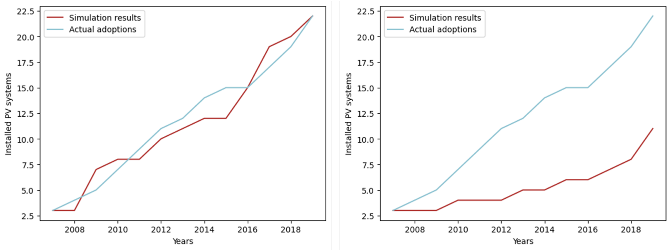

Figure 3. Example of the influence of stochastic elements on the simulation result. Cumulative adoption patterns in two simulation runs of equal parameterization and the reference series. Parameterization is set at an interest threshold of 114 and an adoption threshold of 0.7092.

The approach of operational validation with PVact aimed at finding the parameter combination minimizing the optimization problem of free parameter calibration thus exemplifies a fundamental issue with parameter optimization of stochastic systems. Where differences within runs are significantly larger than differences between (averages) of runs of different parameters, the discriminatory power of performance differences becomes negligible and new approach for model grounding is needed. The model validation approach PVactVal is based on this observation.

IV. PVactVal

PVactVal is a simulation model validation approach that takes into account stochasticity of system dynamics within agent-based innovation diffusion models. Instead of seeing the optimization for a singular parameter combination that minimizes the chosen error metric as a single most parsimonious representation of reality, the approach respects the stochasticity of real-life systems. The approach thus does not evaluate measures or options for action on singular model instances, but groups comparable runs across parameters, stochastic events and scenarios.

The evaluation phase of the modeling process is structured as follows:

1) Define the metric M, parameter range $[\underline{AT}, \overline{AT}] \times [\underline{IT}, \overline{IT}]$[8], granularity $g \in \mathbb{N}^+$ measures $K \ni k_0$ (with k_0 as the reference case (business-as-usual)), and the number of repetitions n,
2) Generate a set of $g^2 * n$ pair-wise different seeds S_L for the random number generator used in the simulation[9],
3) Associate each $i \in [0, g^2 - 1]$ with the parameter combination $(AT_i, IT_i) = (\underline{AT} + ((i \mod g) * \frac{\overline{AT} - \underline{AT}}{g}), (\underline{IT} + (\lfloor \frac{i}{g} \rfloor * \frac{\overline{IT} - \underline{IT}}{g}))$ to create an equidistantly spaced grid of evaluation points within the parameter cuboid[10],
4) For each $k \in K, i \in [0, g^2 - 1], j \in [0, n-1]$ evaluate the model at parameters AT_i, IT_i with seed $s_l \in S_L, l = i * n + j$, yielding model behavior P_{ijk},
5) For each pair $k, \hat{k} \in K$, analyze $M(P_{ijk}, P_{ij\hat{k}})$,
6) For each repetition j aggregate $M(P_{ijk}, P_{ij\hat{k}})$ across $j \in [0, n-1]$ and generate the parameter performance matrix across parameters AT_i, IT_i.

For 1) the modeler should ensure that the used parameter range lies in a plausible region, where the model yield results 'close enough' to the reference data in order to analyze appropriate model instances.

A. Application of PVactVal

In order to apply the PVactVal approach, a small illustrative proof-of-concept study was designed. Within the calibration context of Dresden, scaled down models runs were evaluated with two scenarios k_0, k_1 from 2020 until 2030, which illustrate the influence of the economic parameters. In the reference case k_0, the price degression of PV modules was continued as in the base model, whereas the consumer-side electricity price was kept on the level of 2020 and the feed-in remuneration was moderately reduced by 5% p.a. Based on challenges of a massive need for decarbonization and the energy crises of 2022, in the pessimistic scenario k_1, the residential electricity price was heavily increased by 7% p.a. from 2022 on, along with a linear reduction of feed-in remuneration until 2027 and a slower price degression for PV systems.

Based on the results shown in figure 2, the parameter range of interest was set to $([\underline{AT}, \overline{AT}], [\underline{IT}, \overline{IT}]) = ([0.6, 0.8], [1, 128])$. Tentative results of this small case study with parameters $g = 3, n = 2$ and the mean value as error metric M are seen in figures 4 and 5.

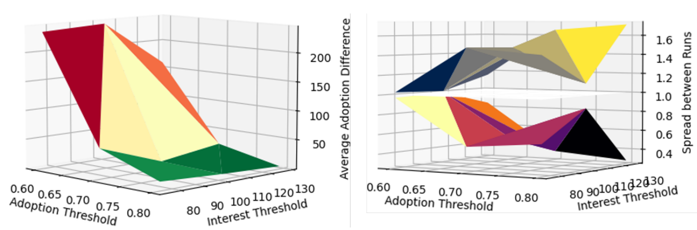

Figure 4. Illustration of the difference of the analysed scenarios. Difference in the absolute number of adoptions throughout the simulation for scenario k_1 with respect to k_0 (left) and the maximal relative spread (top curve) and minimal relative spread (bottom curve) of the different scenario runs (right). For the spread, the maximum and minimum difference in adoption for runs of the same parameter combination was divided by the average spread between the runs. The relative spread thus gives a measure of variability between the runs.

The results demonstrate that the scenario k_1 leads to increased adoptions. They also show that there is considerable

[8]With $\underline{AT}$ as the lower bound of the adoption threshold, $\overline{AT}$ as the upper bound of the adoption threshold, $\underline{IT}$ as the lower bound of the interest threshold and $\overline{IT}$ as the upper bound of the interest treshold.

[9]Two simulation runs with the same seed will yield the same result when parallelism of the runs is deactivated, allowing comparability between runs using the same seed.

[10]This transformation from a one-dimensional index to a two-dimensional grid decomposes the fraction $\frac{i}{g}$ into its whole integer part $\lfloor \frac{i}{g} \rfloor$ (with the floor function projecting a rational number to its lowest integer neighbour) and its remainder (i.e., $\frac{i}{g} = \lfloor \frac{i}{g} \rfloor + i \mod g, \forall i, g \in \mathbb{Z}$).

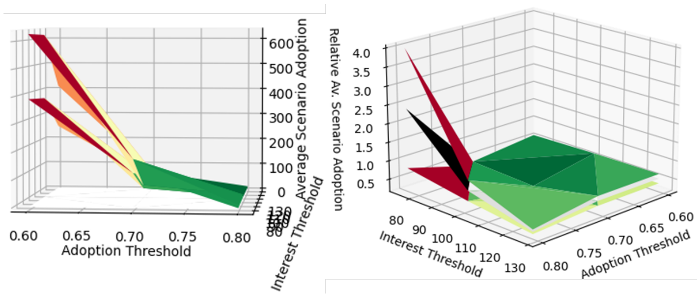

Figure 5. Visualisation of the number of adoptions in the scenarios. Plot of the absolute number of adoptions through the simulation for different parameter combinations (left) and the relative number of cases (right) as normalized by the average number of adoptions in k_0 (top) and k_1.

variation both between runs (as clearly demonstrated in figure 5) and between different parameter combinations. The strong difference in the absolute number of adoption (left plots in figure 4 and 5), particularly for lower adoption parameters, illustrates the different simulation behavior between the two scenarios. The strong variability between different parameterizations, however, shows that the parameter region requires more comprehensive and granular investigation to identify suitable parameter regions. The low granularity was chosen due to the resources constraints in the research associated with this conference paper and was considered to be acceptable as this case-study was presented purely for illustrative purposes with respect to the approach presented above.

While this scenario was designed to be pessimistic for residential consumer agents due to massively increasing electricity cost, it leads to system behavior that, from the aggregated perspective, can be judged rather positively with respect to reaching ambitious decarbonization goals necessary to mitigate the worst scenarios of the climate catastrophe. Due to the cost pressure of **not** adopting, many households adopt the technology, particularly where the burden to adoption (adoption threshold) is low.

For the interpretation of the results, the authors want to stress that these must not be taken normatively, even when considering the need for massive installation of rooftop PV systems. PVact was designed in the context of the modeling infrastructure IRPsim [14] as an agent-based PV diffusion model that was coupled to a techno-economic optimization model primarily used for investigating business models for municipal energy providers. From this perspective, a strong increase in residential power generation by (former) customers, can exert much pressure on these actors. For decision makers in these companies, measures that lead to steep adoption might be judged differently than by other actors.

V. Future Work

The presented research is part of active and ongoing research on the simulation model PVact and is as such part of further investigation concerning the model. Future research will focus on the integration of this validation framework in the deeper understanding of the model. One promising avenue for this is seen in investigating the effect of singular model dynamics on a component-based level. By changing or even switching off certain model components, their effect, as well as the interaction with other model components, can be observed. This would not only inform understanding of the respective components, but the model behavior itself.

Furthermore, model development has focused more on the validation of the model than its application and the evaluation of policy instruments. Implementing the instruments and comparing the inter-instrument differences would lead to insight in both the effects of the instrument and the model. The approach described in IV is explicitly designed to compare different policy measures and should be evaluated through its application to these measures.

On a more theoretical side, further research should analyze different approaches to aggregate the quality of the results. It stands to reason that results differ regarding whether the measures are compared between individual runs (as described in section IV) or if the runs of the same parameter combinations were aggregated before step 5). This would most likely hold as well when the inter-measure comparison is done after the parameter performance matrix is aggregated. This would also depend on *how* the measures are compared. Different runs with different parameter sets lead to a distribution of the model results on which basis the measures are compared. Concretely, this would concern whether the used metrics M are based on a scalar value or a matrix of values and how distances are measured and evaluated.

A further influencing factor on the quality of the results is assumed to be due to the scaling of the computational resources. It stands to reason that the model does not scale linearly and that model behavior would differ qualitatively between the full and the scaled version. A deeper investigation in this matter would be fruitful for the quality of the analysis.

Finally, establishing a stronger link with the literature on uncertainty in modeling and simulation, as well as statistical issues, would prove helpful to anchor the discussion theoretically.

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Parts of this research will further be published in a publically accessible project report on the results of aforementioned project in German [15] (as a chapter in [16]).

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