

# Making Assumptions Transparent: Iterative Exploratory Modeling as a Stepping Stone for Agent-Based Model Development

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**Abstract.** In the case of infectious diseases, the interaction between human behavior and disease dynamics can greatly influence the resulting outbreak size and characteristics. People behave differently depending on the information available, so the influence of local and global information about a virus outbreak is studied. Agent-based modeling provides a tool for representing individual behavioral differences, but its calibration is complex. Several factors influence model results, such as the network structure representing social relationships. Using an exploratory methodology called “Iterative Exploratory Modeling”, the assumptions used for a particular agent-based model are tested and verified, demonstrating the benefits of said approach. While genuine disease dynamics can be achieved with the used graph based on the Barabási-Albert model, the specific graph attributes have a much larger impact on the results than the local and global information. This emphasizes the need for testing assumptions at a fundamental level, which “Iterative Exploratory Modeling” can provide.

**Keywords:** Information · Dynamics · Simulation · Agent-Based Modeling · Multi-Agent Simulation · Epidemiology · Social Networks · Graphs · Network Aspects · Social Influence · Local vs. Global Information

## 1 Introduction

The impact of pandemics on human life has become apparent in recent years. In particular, the interdependence of human behavior and disease dynamics has become a research focus. Sometimes referred to as “coupled contagion” [12], individual protective behavior is a function of risk perception and thus influences the spread of disease over time. In addition, the state of the disease spread also influences risk perception, creating a feedback loop. This effect is often abstracted in traditional modeling, especially compartmental modeling, leading to an incomplete representation of some driving forces behind disease spread. Agent-based modeling is useful for this coupling of behavior and disease spread.

The heterogeneity of the agents in a model allows behavioral changes to occur based on the effect of receiving information. This paper uses an exploratory approach called “*Iterative Exploratory Modeling (IEM)*” to understand the underlying assumptions that generate different model results. Therefore, *IEM* aims to test the assumptions’ validity, especially regarding the graph used to represent the social network. *IEM* makes the assumptions transparent, showing eventual dependencies on the model results. The goal is to transform the process of agent-based modeling into a method that is easier to understand.

## 2 Preliminaries

One of the best analogies to the principle of agent-based modeling comes from biology, from the field of swarm intelligence. Here the basic insight is as follows:

“Complex collective behavior can emerge from individuals following simple rules”. [5, p. 110]

This paper uses the terms *agent-based modeling*, and *agent-based model*, *ABM* is used as a shorthand for both terms. An *agent-based modeling* is a simulation involving many agents’ interactions. Simulation, in this case, refers to the concrete execution of the code in which the modeling is implemented, while modeling refers to the conceptual level. This interaction follows defined rules; the agents and the space they interact in have defined properties. The goal of the simulation is to study the outcome of the interaction of the agents based on these defined rules and constraints.

### 2.1 Use Cases of *ABM*

*ABM* can be used to pursue entirely different goals. The purpose of modeling is not always to predict phenomena or values; *ABM* can also describe these phenomena or explain their mechanisms. Wilensky and Rand define eight different use cases for *ABM*:

say(1) description, (2) explanation, (3) experimentation, (4) providing sources of analogy, (5) communication/education, (6) providing focal objects or centerpieces for scientific dialogue, (7) as thought experiments, and (8) prediction [20, p. 28].

An experimental approach can facilitate the understanding of a complex system. If the model is built according to the known properties, new parameters and rules can be easily inserted, whose influence can be successively determined by analyzing the simulation results [20]. Thus, one of the conclusions from the previous paragraphs is that even very simple models can yield surprising results. Especially in the social sciences, the goal of an *ABM* is often an understanding of the system’s interrelationships and the parameters’ effects. Therefore a reality-based representation is less important [13,6].

## 2.2 Epidemiological Basics

The theoretical foundations of epidemiology are highly relevant to modeling the spread of an epidemic. The importance of this area of research has become apparent to the general public in recent years, as the COVID-19 pandemic has caused drastic changes in many areas of personal and public life.

Epidemiology and social sciences are usually considered separately, but it is crucial to consider and use findings from both fields when studying pandemics. The example of the COVID-19 pandemic shows the substantial impact on social science issues such as individual protective behavior or social solidarity. Even before that, infectious diseases such as HIV have always had and continue to have a major impact on global sociopolitical issues [11]. Demographic parameters also play an essential role, as the risk of contracting the disease may depend not only on genetic factors but also, for example, on age [17].

This paper uses a basic Susceptible-Infected-Recovered (*SIR*) model. The key indicators that are discussed in this paper are incidence and prevalence. The maxima of the respective numbers of persons who can be assigned to a specific condition according to the *SIR* model are suitable as other critical figures for investigating the spread of an epidemic. That is, the maximum of infected persons and the maximum incidence are apparent values to classify the epidemic. Furthermore, the duration of the infection period in the case of a temporally limited spread of infectious disease and the proportion of persons who were never infected after the end of the epidemic are meaningful [18].

## 2.3 Social Networks

The social network, i.e., the network of interpersonal relationships of a human being, can be represented by graphs. Typical approaches include random networks produced by generative models such as the Erdős-Rényi model and so-called *small world* networks generated by the Watts-Strogatz model. Scale-free networks can be built using the Barabási-Albert model, and the resulting graphs are referred to in this paper as *BA* graphs. The latter has been established for mapping *Social Networks* in the context of epidemiology because they resemble many real-world networks. An example is the study of the number of sexual partners, where Liljeros represents the mechanism of a scale-free network [2,15,16,9]. However, mapping a *social network* by a *BA* graph is also criticized because some assumptions are too simple. Moreover, Jin and Yu also note that most networks are weighted in reality, which is not valid for any of the presented graphs [19,14]. With *IEM*, I aim to make the influence of these assumptions more apparent.

These networks are created iteratively in the case of the *BA* graph, following a principle of *preferential attachment* that is often described as “the rich get richer” [16]. Thus, the graph starts with a certain number of nodes with connections (edges) between them, to which new nodes are added. The existing node with the most edges has the highest probability of forming edges with the newly added nodes. The result is a graph in which a few nodes have a very high number of edges, but most nodes have very few edges. Thus, a scale-free network also

exhibits the property that defines *small world* networks, namely a small number of steps required to move from node to node, starting from a starting node to any other node.

In epidemiology, this means that scale-free networks such as the *BA* graph show a very rapid spread of infectious diseases - but this also makes them more sensitive to isolating the few nodes that cause many infections. These nodes thus correspond to the "super-spreaders" that were also a problem during the COVID-19 pandemic [3,15,16].

## 2.4 Research Question and Assumptions

The concept of *Iterative Exploratory Modeling*, introduced in the next chapter, does not involve traditional research questions from which I derive testable hypotheses. Instead, I subsume the focus of the investigation under this more open research question:

How do behavior changes due to information gain affect the overall epidemiological picture?

The focus here is on the impact of modeled parameters on infection incidence. Specifically, information about the epidemic situation should induce a change in agents' behavior, and I will examine the extent of different levels of risk reduction. This information can be at the global level (equivalent to information from official sources such as government agencies or the media) or at the local level (through information exchange with other agents or using a contact tracing app). Moreover, the impact of vaccination effectiveness and isolation will be analyzed.

As described above, the formulation of assumptions instead of hypotheses could be more useful. Therefore, I will test two basic assumptions. The first of these is

*An increase in the number of infections leads to a behavior of minimizing the risk of individual people.*

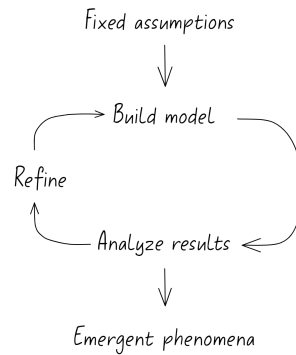
The second reads:

*Risk minimization of individual agents reduces the spread of the epidemic and decreases its ultimate magnitude.*

## 3 Iterative Exploratory Modeling

I follow an unconventional and open approach called *Iterative Exploratory Modeling* in this paper. Wilensky and Rand define *Exploratory Modeling* as the second overarching category of modeling [20]. This method is an advantage of agent-based modeling because it allows a model to be built to explain observed phenomena. I create a model from initially chosen parameters, the results of this model are analyzed, and I progressively approximate the model to the observed phenomenon.

I explicitly extend this concept by an iterative approach called *Iterative Exploratory Modeling*. It represents a partially cyclical process in which I make basic assumptions, which are not changed, and from which I generate a model. This model then produces results through simulation, which are analyzed to discover emergent phenomena. I extend the model progressively and then re-examine the results (see fig. 1). I do not change the original assumptions, but the model and the parameters used can be modified. Parameters may also be added or removed. This process continues, ideally, until emergent behavior is discovered.



**Fig. 1.** Iterative Exploratory Modeling

### 3.1 Model

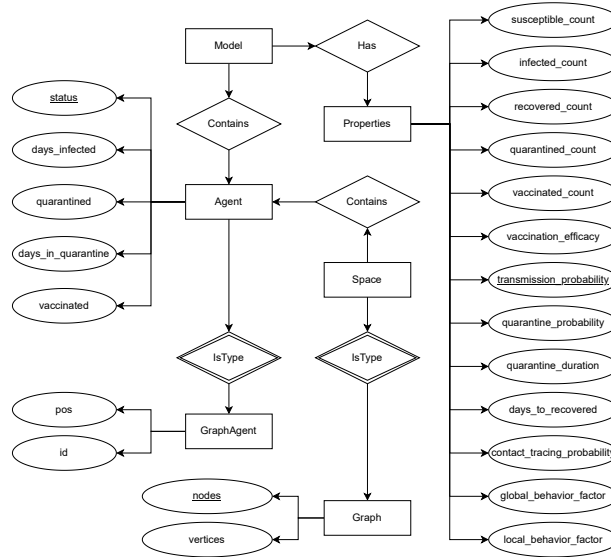
I will now demonstrate the Iterative Exploratory Modeling approach using the model I introduced in the previous chapter. Fixed assumptions are:

- Individual agents
- Graph as space
- *SIR* model of certain complexity

These three main assumptions establish the following details: Agents represent individuals with specific attributes that may vary from person to person. These agents are located in a graph representing the *social network* of individuals. Through a *SIR* model described in section 2.2, I model the infection event where there are at least three states *Susceptible*, *Infected*, and *Recovered*. An agent can only be in one of these states at a time. The agents can interact with each other and behave dynamically.

The basis for the agent-based model is the framework *Agents.jl*, available for the programming language Julia [8,4]. For this work, I use Julia v1.5.4 and *Agents.jl* v4.5.6. The advantage of this framework is the ease of use, but the high performance compared to other frameworks is also highlighted [1].

There are also three components to the basic structure of *ABM*. The concrete model has properties that partly determine the model’s functioning or are used to collect the results. The agents, which are part of the model and are located in the space, also have properties, but these only affect the individual agent. Finally, the space has properties that define the type of space and its concrete nature. The fig. 2 overviews the relationships between the components and their properties.



**Fig. 2.** Entity relationship diagram of the model used. It shows the components of the model and their properties, as well as the relationships among them.

In the *ABM* presented here, the configuration defines the fixed properties of the model and the default parameters. These are the total number of agents (which corresponds to the number of nodes in the graph), a parameter defining the *Preferential Attachment* used to create the *BA* graph, the number of steps (days) for which the model should be simulated, and the default parameters.

I use these default values unless other values or ranges are defined in the list of parameters. They are partly based on the chosen maximum values for the parameter ranges investigated in this work and partly on a realistic assumption. For example, I assume an isolation period of seven days and an infection period of 14 days can be assumed. The transmission probability, on the other hand, is chosen intuitively and then adjusted to a realistic spread by approximating the *SIR* model. To reiterate, the focus of this paper is to demonstrate the use of *Iterative Exploratory Modeling*, meaning that realistic parameter values are not always needed. Instead, the idea is to test the validity of these intuitive assumptions. I approximate vaccine effectiveness to be 80% based on the average

effectiveness of all COVID-19 vaccines relative to the delta variant. The probability of contact tracing is also adjusted to a realistic number based on the number of devices on which the application is installed. The values for the local and global behavioral factors are based on the assumption that infecting all people within a person’s radius will cause them to change their behavior, ultimately halving the risk of infection. The global behavioral factor assumes that even if the entire population is infected, the risk of infection is reduced by no more than 25%. I make this assumption intuitively and discuss the implications of this assumption in section 4.1.

The values for these are:

- Total number of agents (number of nodes): 1000
- Number of connected nodes and new connections a newly added node has: 3
- Number of steps (days): 150
- Isolation duration: 7 days
- Vaccine effectiveness: 80%.
- Transmission probability: 20%.
- Probability of contact tracing: 50%.
- Isolation probability: 0%.
- Duration of infection/number of days until transition to *Recovered*: 14
- Local Behavioral Factor: 0.5
- Global Behavioral Factor: 0.25

I define the effectiveness of the vaccination by *vaccination\_efficacy*, which can take values between 0 and 100 (%). This corresponds to a reduction of the probability of transmission by this percentage. I define the transmission probability of the infectious disease by *transmission\_probability*. This value can range from 0 to 1 and is the factor used to model the risk of infection. The *quarantine\_probability* property defines the probability that an infected agent will be quarantined and can range from 0 to 100 (%). Due to a terminology error, I defined this parameter as quarantine. The correct value is “isolation”. I perform the check to see if an agent goes into isolation each day the agent is infected. This increases the probability of an agent going into isolation from day to day. I intend this modeling to reflect that infection is usually not detected immediately but may be detected several days after the initial infection. In some instances may never be detected. Thus, assuming a defined isolation probability of 10%, the total probability of an agent going into isolation is calculated to be approximately 80% for an infection period of 14 days. *quarantine\_duration* denotes the duration of isolation, *days\_to\_recovered* the duration of infection or the number of days after which an agent changes from *infected* to *recovered*.

To represent behavioral changes, two factors represent the reduction in risk of infection due to increased hygiene measures or social distancing. These factors can take values between 0 and 1, with 1 representing a complete reduction in the risk of infection. Specifically, the global behavioral factor refers to the mechanism by which increasing numbers of infections among the total number of agents leads to behavior that minimizes the risk of individual agents. I define the number of infections among the total number of agents as global information intended

to represent, for example, media reports or notifications by authorities. The local information, which influences the local behavior factor, is defined as the number of infections in the agent’s neighborhood. Here, the agent’s neighborhood denotes all neighbors, i.e., directly connected nodes, that the agent has according to the *social network* modeled with a *BA* graph. However, to represent that an individual agent is unaware of every infection of its neighbors, I define a probability called *Contact Tracing Probability*. This determines the fraction of infections in its neighborhood the agent is informed about. Conceptually, I model this approach using a contact tracing app, such as the “Corona-Warn-App”. The probability that the agent’s neighbors use this app results in a fraction of neighbors whose infection the agent is informed about. Thus, this parameter directly affects the Local Behavioral Factor and can also be considered a factor for the strength of the effect of local information. Therefore, if a local behavior factor of 0.5 would mean a halving of the risk of infection for a *Contact Tracing Probability* of 100%, this would only mean a 25% reduction in risk for a *Contact Tracing Probability* of 50%.

The parameter ranges studied in this paper are as follows:

- Vaccination Efficacy: 70%, 80%, and 90%.
- Isolation Probability: 0 to 10% in 2.5% increments.
- Contact Tracing Probability: 0 to 100% in 10% increments.
- Local Behavior Factor: 0 to 0.5 in increments of 0.1
- Global Behavior Factor: 0 to 0.25 in 0.05 increments

After defining the parameters to be simulated, I initialize the model with the specified configuration and the chosen parameters. Here the graph representing the *social network* is created, where an agent is assigned to each node in a second step, leading to the nodes representing the agents. Exactly one agent with the state *Infected* is always inserted into the graph at the node with the highest node degree. This node has the most connections to other nodes, leading to a fast infection spread. I also chose this step to guarantee the spread of the infectious disease since if the number of neighbors is low or the agents have no neighbors, the spread may die after a very short time or never spread. The nodes with no neighbors represent individuals who live in complete isolation and, therefore, can never be affected by the infection.

## 4 Summary of Results and Discussion

With the default parameters, a reasonable representation of an epidemic is achieved by the implemented *SIR* model; the trajectory of infection numbers corresponds to the typical trajectories given in the literature. Adding vaccination to the *SIR* model increases the sophistication of the model, but the effect of different levels of vaccination effectiveness is small. Adding isolation adds a parameter to the model with a substantial impact on infection spread.

Certain key figures and parameters are abbreviated as follows:



- *Susceptible Fraction Remaining (SFR)*: Proportion of agents with *Susceptible* status at the endpoint of the simulation, equal to the proportion of agents never infected.
- *First to Last Infected (FTLI)*: Number of time steps between the first and last time an agent exhibited the *Infected* status, this maps the 'width' of the infection curve.
- *Day of maximum Incidence (DomInc)*: Time step with the highest incidence
- *Day of maximum Infected (DomInf)*: Time step with maximum number of agents with *Infected* status.

The effect of isolation probability is most evident in the number of maximum infected agents and the proportion of agents that were never infected at the end of the simulation (*SFR*). Increasing the isolation probability results in a large decrease in these metrics. Increasing the *Contact Tracing Probability* leads to a reduction in the size of the epidemic in the form of a reduction in the maximum number of infected or an increase in the proportion of agents never infected at the end of the simulation. This effect is evident when considered without isolation, but it is a weaker reduction than for isolation probability. A higher *Contact Tracing Probability* at the maximum local behavior factor leads to a significant decrease in the maximum number of infected at low isolation probabilities. However, as the isolation probability increases, this effect diminishes because it is masked by the significant influence of the isolation probability. The local behavioral factor leads to a weak reduction in the size of the epidemic as a function of the *Contact Tracing Probability*, which is not as strongly influenced by the isolation probability. The global behavioral factor leads to a very weak reduction even without isolation. The effect of all parameters on the metrics *FTLI*, as well as *DomInf* and *DomInc* is very small or non-existent. These results are discussed in the next section.

#### 4.1 Discussion

In this section, I will first discuss the issues arising from the specific model I implemented. I will then discuss how these issues relate to the Iterative Exploratory Modeling approach.

One of the issues found in retrospect is that an insufficient implementation of vaccination leads to low immunization influence on the model results. There is a fixed probability that agents can enter the *Vaccinated* state at each time step. This results in a linear trend for the time period presented here. At the time of maximum infection, the proportion vaccinated is approximately equal to the proportion infected. At this time, only about a quarter of the agents are protected by vaccination, which explains the weak effect. *IEM* has two benefits here: For one, the model in its current state demonstrates the considerable influence of the protection granted by vaccination on disease transmission which is in itself a key result. If I take the IEM approach further, I could adjust the vaccination implementation and compare model results to the previous state.

Another key finding of this exploratory approach is the strong influence of the

graph used to represent the social network. One of the implications of this finding is that isolation strongly influences the model results. The argument is that due to the small number of highly connected nodes, it is sufficient for one or more of these nodes to become isolated and significantly hinder the spread of the disease. Due to the high variation between runs as a result of the different graphs, this emphasizes the need for calibration and batch runs. Another possibility would be to keep the graph used for simulation fixed.

An additional problem with scale-free graphs is the lack of homophily, which can significantly affect network clustering and the disease dynamics. Another problem is that static networks cannot represent the dynamic processes in human relationships, such as forming and terminating connections [18,15]. Therefore, the *IEM* approach allowed me to discover an influence on model mechanics that was also discussed by [18,15].

The type of graph used to map the social network significantly impacts the spread of the virus. *FTLI* represents the number of steps between the first and the last infected agent, so it also describes the "duration" of the spread. The spread of the virus in the concrete *BA* graph may always be very uniform. That is, the maximum number of infected and therefore *SFR* is independent of the 'duration' of the infection period. Even if more agents are infected, the virus does not spread 'faster' than if only a few agents are infected. This may be due to the *small world* properties of the *BA* graph. Also, the small size of the graph used may have unintended consequences. With a relatively small number of agents (1000) and a relatively small average path length, propagation within the chart might be very uniform, regardless of the number of infected agents. This effect could be further analyzed by increasing the number of agents or by examining the properties of the graph more closely.

Because of its implementation, the *Contact Tracing Probability* is, in fact, only a reinforcement factor for the local behavioral factor. With a *Contact Tracing Probability* of 0%, the local behavior factor does not affect reducing the transmission probability; with a *Contact Tracing Probability* of 100%, it has a significant effect. This explains the dependence of the two values. The influence on the number of infections can be explained by the fact that the local behavior factor of 0.5 is less limited upwards than, e.g., the global behavior factor of 0.25. In addition, the local behavior factor is related to infections near the agent. There, the entire perimeter can be infected proportionally faster. The global behavior factor, associated with the number of infected people in the total number of agents, is usually lower. The strong influence of these two effects on the metric shown is due to their interaction.

The small effect of the global behavior factor can be explained by analogy with the strong impact of the local behavior factor. On the one hand, the maximum value of the global behavior factor is limited to 0.25, i.e., it can only reduce the risk of infection by 25%. In addition, this effect still depends on the proportion of infected people, which rarely exceeds 50%. In the best case, the transmission probability is reduced by 12.5%. Since the ratio of infected persons is typically closer to 25%, the small effect due to the definition is obvious.

## 4.2 Benefits of Simple Models

*ABM* are also suitable as an introduction to a complex topic because of their explicit modeling of parameters. One perspective on this model, not only because of the approach of *Iterative Exploratory Modeling* (defined in section 3, is to see it as a starting point for the investigation of a phenomenon. Therefore, if discovered, inconsistencies or methodological errors are always an opportunity to improve the existing model. This is especially true in the iterative context of Iterative Exploratory Modeling, where this work can be a valuable starting point for further investigation. Another insight from section 2 is that even simple models can produce interesting results. Thus, increasing the complexity of the model is no guarantee that the results will be more relevant. Therefore, it should be mentioned here that “simple” is not necessarily “bad”.

In this sense, the requirement that an *ABM* should always add value for application in the real world is fulfilled [7]. At least if this added value, as according to Epstein and Bruch&Atwell, also lies in reviewing the assumptions and simplifications underlying a model, raising new questions, working out ambiguities, and highlighting advantages and disadvantages of these aspects [10,6].

## 4.3 Verification of Assumptions

The basic assumptions of the model concern the representation of *Social Networks* as *BA* graphs, the simplification of behavioral changes as a direct reduction of the transmission probability, and the representation of agents as nodes, as well as the restriction of the *SIR* model to a very simple implementation.

The model’s representation of typical *SIR* curves, described in section 4, confirms the first assumption. Thus, *BA* graphs are suitable for representing *Social Networks* in the context of an *ABM* model integrated with an *SIR* model. However, it should be emphasized that the properties of the graph significantly impact the results of the *ABM*. Therefore, one of the most important findings of this work is the importance of studying the influence of the graph used on the *ABM*. The precise definition of the properties of the graph contributes significantly to the results of the *ABM*. The second assumption that the effect of behavioral changes can be directly implemented as a reduction in transmission probability must be viewed critically. Although it was found that the second assumption was confirmed, the influence of the psychological process in the background is not represented in this way. Perhaps a better representation of human behavior by a simple behavioral model is needed here. The representation of agents as nodes and that of the simple *SIR* model, at least to achieve a qualitative similarity of *SIR* numbers to observed data, can be interpreted as permissible based on the results.

## 5 Outlook and Further Work

Further iteration steps, which are conceivable in the context of *Iterative Exploratory Modeling*, but which I could not implement in this work, are presented here.

## 5.1 Further Iteration Steps

Additional attributes could be added to the agents to achieve more realistic heterogeneity. So far, this is only represented by probabilistic behavior, which has drawbacks. An age-dependent transmission probability could be introduced, or similar to Kitchovitch and Liò, a perception of perceived risk [15]. This could be a good guideline for implementing more complex behavior. This behavior could also be made dependent on the individual characteristics of the agent, which would allow a complete mapping of a behavioral change. This behavior could be adapted and influenced by interaction with other agents. The interaction could be modeled by building a perceptual model that stores an interaction history and uses it to adjust the properties of the agents. This perceptual model would also be a step towards implementing deterministic behavior. Another iterative step could be to implement a spatial model that better represents specific effects of infection risk and daily life. A spatial model would also expand the possibilities for interaction between agents. In addition, simulation steps could be defined on a smaller scale to allow for more dynamic processes. Finally, an adaptation of the *SIRV* model could be considered to accurately model the willingness to vaccinate, which increases with an increasing number of infections or certain behaviors. Finally, the possibility of re-infection with the virus could be included.

## 5.2 Outlook

The main result of this work is to highlight the validity of the assumptions made in the modeling process. This includes the verification of the mapping of *Social Networks* by a *BA* graph, a reduction of the behavioral model to a direct influence on the transmission probability, and the use of a simple *SIR* model. Using a *BA* graph in combination with the *SIR* model is valid for studying the spread of an epidemic. Reducing the behavioral model is helpful for a basic understanding, but I recommend an extension with a simple behavioral model. Incorporating risk perception could make the behavior deterministic and thus reduce the randomness of the model.

Understanding complex systems is relevant in many fields, and the interaction of epidemiology and human behavior is complicated. Using an unconventional and open-ended approach called *Iterative Exploratory Modeling*, the goal is to understand and explain the underlying mechanisms of a model. I based this modeling on a combination of the approaches of *Agent Based Modeling* and a *SIR* model. The latter is suitable for creating a sufficiently accurate abstraction of the processes under investigation, which I used to test various assumptions. This way, an understanding model can be built iteratively, covering different levels of complexity. This process results in a model that can be a starting point for further research. The conditions for a more comprehensive view of the phenomena are justified by testing the critical assumptions of the model. The contribution to the understanding of epidemics and human behavior made in this work should therefore contribute to reducing the risk and magnitude of future epidemics.

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