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Origin and Goal of Computational Experiments

This chapter clearly states that the core of computational experiments lies in "generative explanations." It studies social complexity from the bottom up, based on mathematical modeling of micro-level agents, using computer simulation techniques to derive the macro-evolutionary process of social systems and by designing experiments and causal inference methods to explore the underlying rules behind phenomena. Computational experiment method represents a higher level in computational simulation technology, offering a feasible way to analyze the behavior of complex systems and evaluate the effects of various decisions. It also bridges the gap left by traditional methods, which struggle or fail to experiment on complex systems.

1.1 Complexity Science

1.1.1 Basic Concepts of Complexity

Prediction is the oldest endeavor of mankind. From an individual's fate, including birth, aging, illness, and death, to the rise and fall of a country, all fall within this vast realm of prediction. Imagine if you could predict one's life, or if someone could predict the rise and fall of a country or even humanity, how significant that would be. Asimov's novel *Foundation* once depicted such a scenario. One Hari Seldon invented the science of "psychohistory" and was able to predict the rise and fall of the entire galactic empire. If we roughly classify the things in this world, we can divide them into two major categories: one is called "inanimate things," such as stars, solids, liquids, various molecules, atoms, and subatomic particles in the universe, and the other is "living things," including everything related to life, from various biological cell processes to neural activities in the brain to social and economic systems. For the first category of things, we have achieved highly successful predictions, while the second category is fraught with difficulties.

In the process of scientific development, scientists once viewed the universe as a mechanical clock, believing that as long as they understood the laws that govern the universe, they could infer the past and predict the future. Laplace once wrote: "If a wise man can analyze all the data of the natural world, he can put the movement of the largest celestial body and the smallest atom in the universe into a single formula. For such a wise man, nothing is uncertain, and the future is as clear as the past." The evolution of the planetary motion model is a classic example of this kind of deterministic prediction. At first, Ptolemy's cosmic model decomposed the movement of the sun, moon, and stars into a series of mutually nested circular motions; second, Copernicus proposed the heliocentric theory; third, Kepler turned circular orbits into elliptical orbits; and, finally, Newton transformed empirical theorems into a theoretical system and proposed Newtonian mechanics represented by differential equations. These theories can predict changes in various phenomena and can be tested by experiments. From the parabola of an apple falling to the ground to the movement of the sun, moon, and stars, they are all unified. This method of decomposing phenomena and abstracting the most general factors is physical thinking.

Soon, this deterministic thinking began to enter the microscopic world. Due to the uncertainty principle, these tiny particles have inherent uncertainty. If the motion of atoms is random, then why are the macroscopic substances they form, which have temperature, hardness, shape, and chemical properties, determined? Can we predict the macroscopic from the microscopic? This time, this is made possible by statistical physics, whose core idea is that although the movement of a large number of particles at the microscopic scale is random, the characteristics at the macroscopic scale obtained through statistical methods are stable and predictable. For example, we can calculate the magnetism of a magnet and the boiling point of water. The law of large numbers explains how random microscopic behavior yields predictable macroscopic phenomena. The key to the law of large numbers lies in the continuous addition of countless random and independent variables, which will result in a deterministic entity on a larger scale.

People used to be optimistic, thinking that they had understood the world and had given a perfect description of the world with mathematics. However, this optimism was short-lived. By the 20th century, with the rise of the Internet and big data, humanity's mathematical prediction ability has once again been unprecedentedly enhanced. People began to think further along the same lines as before: Does society itself also have first principles similar to Newton's laws, and can it be predicted using statistical physics? Such a desire is vividly described in Asimov's "Foundation": "Each member of human society is like a molecule in a gas. Their movement may be random and unpredictable, but the human society they form is highly predictable." Therefore, this science predicted the decline of the entire galactic empire, thus launching the entire plan to change human history. This is simply a reiteration of the view of statistical physics. Each person is random and unpredictable, but when a large number of people are considered collectively, the rise and fall of a country or a nation is highly predictable.

However, people soon discovered that the world is actually highly complex, especially in areas related to people or society, and the predictions made have largely gone unfulfilled. There is an interesting social experiment: "If the number of people in a group is fixed, everyone starts with 100 yuan, then plays a game, and each person randomly gives 1 yuan to the people around them; if this chain of funds is passed on in this way, then after a period of time, there will be a distribution of the funds of the people in the group; what kind of characteristics will this distribution take?" According to statistical physics, this process should be close to the physical diffusion process and thus result in a classical Boltzmann distribution. However, this is not the case. In fact, this distribution is much more extreme than the Boltzmann distribution, exhibiting a power-law distribution. Another typical example of prediction failure is the financial crises and stock market fluctuations. The essence of stock market prices is people's expectations of a company's total value in the future, which is determined by a large number of traders who engage in buying and selling. If these traders were like the particles that make up a material entity, behaving randomly but statistically predictable, then the market as a whole would conform to a classic stochastic differential equation. However, the reality goes against the original expectations of the geniuses. So many people entered the stock market to trade and compete, but few could have predicted the financial crisis in 2008 (Figure 1.1).

The German psychologist D. Dörner once raised a question: assuming that people have all the necessary intelligence, experience, and information conditions, why do they still make mistakes, sometimes even with disastrous consequences?

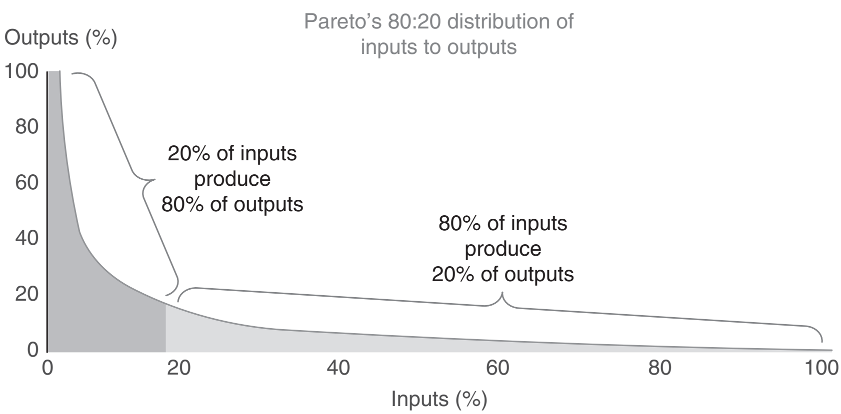

Figure 1.1 The cruel reality and the failure of statistical physics.

In his book entitled *The Logic of Failure*, he gave his own answer [1]: some of people's thought patterns are suitable for a simple world but have a disastrous impact on the complex world they live in. Derner found many examples, such as the planners of the Aswan Dam who only thought of the benefits of cheap electricity for Egypt, but did not realize that this would also interrupt the annual flood irrigation, which has maintained the fertility and prosperity of the Nile Valley for thousands of years. People reclaimed wasteland in the hope of increasing food production but failed to realize the need to protect the ecosystem, which ultimately led to land desertification and food failure. All these show that taking action before understanding all the interconnected factors in a complex system is bound to make big mistakes even if the original intent is good; small mistakes accumulate and eventually lead to serious mistakes; those who too often ignore the overall situation of the problem and only seek expedients in a local area can only be a drop in the bucket and will not help.

For human society, the independence assumption of statistical physics does not hold. The development of human society is closely related not only to its initial conditions but also to random events in its development process. A slight change in the initial conditions will lead to a huge deviation in the final results. In order to avoid failure to the greatest extent possible, it is necessary to understand the laws governing the operation of social complex systems. As J. Achenbach pointed out: "Science is gradually moving out of the field of easy-to-solve problems and beginning to touch on truly difficult problems. Science has reached a new turning point." Since the mid-1980s, some visionary scientists have begun to explore this new turning point, and a discipline known as the "science of the 21st century," complexity science, has emerged [2]. In April 1999, the American magazine *Science* published a special issue with the theme of "complex systems," reporting on complexity research in chemistry, biology, neurology, physical geography, climatology, economics, and other fields. As shown in Figure 1.2, complex systems have some common characteristics: a system exchanges matter, energy, and information with the external environment. Under the joint action of external stimuli and internal drives, the mutual influence between individuals cannot be ignored. System complexity will give rise to the following effects:

1.1.1.1 Nonlinear

The development of phenomena is not isolated, fragmented, or unconnected, but a unified whole that is interconnected, interactive, and mutually constrained. The characteristics of an organization do not depend only on the characteristics of individual components but also on how the individual components are interconnected to form an organization. The interaction makes it difficult to divide the system into parts and thus makes the overall characteristics difficult to predict, which is also called nonlinearity. The basic types of nonlinearity include negative feedback and

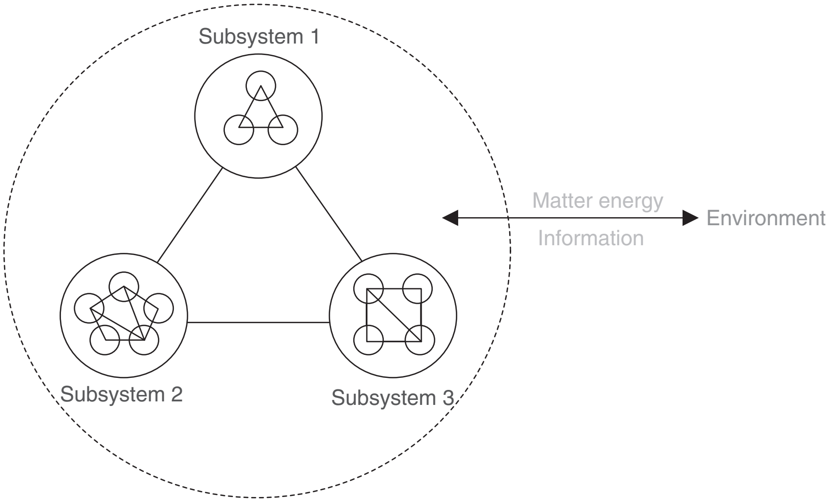

Figure 1.2 Schematic diagram of a complex system.

positive feedback, which make the result of the whole being more than or less than the sum of its parts, that is, $1 + 1 > 2$, or $1 + 1 < 2$, but basically not $1 + 1 = 2$. There are many such examples around us. A team composed of a group of excellent players may make mistakes repeatedly, while a rabble can succeed under a clear set of rules. Nonlinearity means opportunity for ordinary individuals. Due to continuous positive feedback, a single node can sometimes change the entire network, similar to how an ordinary individual sometimes suddenly changes the course of history.

1.1.1.2 Chaos

Weather forecasting has always been an important topic in agricultural production. Physicists once believed that as long as the fluid mechanics equations of gas motion can be solved, the weather one month later can be predicted through a large number of simulations. However, in the process of meteorologists trying to model the atmosphere, they discovered an incredible phenomenon: for the same data, if one more decimal place is retained, the calculated result is sunny; if one less decimal place is retained, the calculated result is rainy. This physical phenomenon is called "chaos." Chaos is caused by the increase in free dimensions in the system. The dynamic properties of the system are no longer confined to closed orbits, but open or unpredictable trajectories. The impact of slight changes in initial conditions on the future is far from known. Most nonlinear networks are in the conditional range where chaos occurs, which makes certainty gradually fade from our view. When the positive feedback in the nonlinear network reaches a certain level, it will transition from a relatively stable structure to chaos. This point on the edge of chaos is called the phase transition point, which is the foundation for the emergence of all complex structures (order).

1.1.1.3 Phase Transition and Emergence

Subsystems and elements within the system interact in various modes and exchange resources with the external environment, thus changing the internal structure and system behavior. After various external information, materials, and so on enter the system, the internal elements constantly collide and react with each other. After a certain period of amplification and development, new forms and characteristics will emerge as a whole, resulting in emergence. Emergence reflects the relationship between the macro and micro levels and is the macro effect of the micro behavior of complex systems. Phase change is the process of causing the entire system to transition from one phase to another through external variables. Taking the phase change from water to ice as an example, the controllable external variable is temperature. When the temperature is 0 °C, the system has the minimum degree of freedom and is in a uniformly ordered state; as the temperature rises, the degree of freedom of the disordered state gradually increases; at a certain temperature, disorder and order alternate, and this temperature is called the critical temperature. The so-called critical state is the state at the time of phase change, because this moment is the most distinctive. Emergence and phase transition points are also inextricably linked. Interested readers can refer to the theory of self-organized criticality.

1.1.1.4 Feedback Loop

When studying the evolution of a complex system, we often need to consider the impact of the current results on the system's output at the next moment. According to Jones's classification of the emergence mechanism of complex systems, emergence featuring a two-way feedback mechanism (feedforward and feedback) between the system as a whole and individual behavior is called second-order emergence, and the emergence with only a one-way feedback mechanism is called first-order emergence. As shown in Figure 1.3, all emergence in social complex systems belongs to second-order emergence: individual behavior generates new individual behavior due to system feedback; complex systems introduce feedback that affects individual behavior on the basis of the original first-order emergence, thus forming a two-way feedback loop within the system, and increasing the complexity of the system. Feedback is divided into positive feedback and negative feedback: negative feedback leads to a fixed-point equilibrium; for example, market prices always fluctuate around the equilibrium level, high prices lead to fewer consumers, and fewer consumers lead to lower prices; positive feedback leads to instability, such as avalanches and stock market crashes.

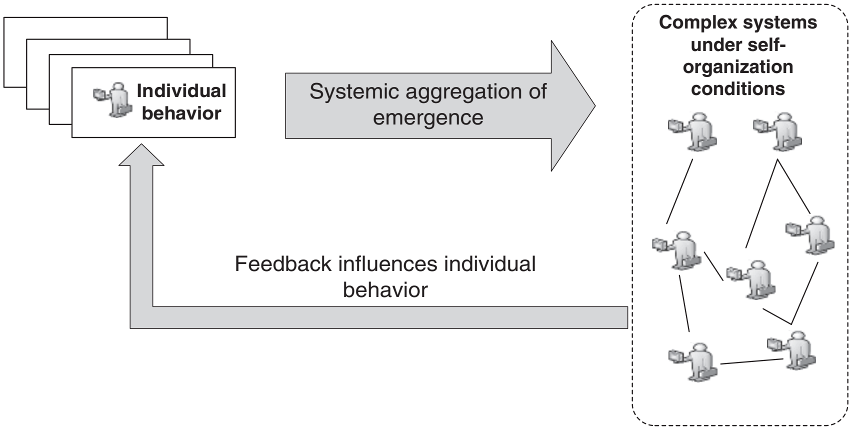

Figure 1.3 Schematic diagram of second-order emergence.

System complexity is the dialectical unity of diversity and consistency. Diversity refers to the heterogeneity of system composition and is also the basis for the system's vitality, creativity, and evolutionary ability, while consistency is the basic condition for the system to form a certain order and function. Studying social systems from the perspective of system complexity focuses more on the diverse behaviors of heterogeneous subjects and the dynamic equilibrium process of interconnection and interaction between heterogeneous subjects. This perspective of system complexity, which emphasizes the dialectical unity of diversity and consistency, helps to deeply understand and grasp the evolutionary and regulatory laws of the unity of "order and vitality" of the system and to overcome the limitations of traditional research methods, such as localization, linearity, and static analysis. Although we cannot accurately predict the behavior of each individual or even society, we can still make correct decisions.

1.1.2 Complex Social System: Cyber, Physical, and Social System

Nowadays, intelligent technologies are developing rapidly. Related technologies include information and communication technologies such as the Internet of Things (IoT), big data, cloud computing, virtual reality, blockchain, and artificial intelligence (AI). Moreover, new technologies or products are constantly emerging. Human society is like a container, within which these intelligent technology clusters are constantly undergoing various combinations and integrations to form various services that meet complex application scenarios [3]. "Data + computing power + AI algorithms" is forming a new type of infrastructure for an intelligent society. Based on this, the entire society is gradually evolving into a complex functional entity that matches demands with services. It is jointly created and operated by all members of society. Driven by data logic, it achieves iterative evolution and self-growth and possesses energy and vitality beyond imagination [4]. The term "intelligent" in an intelligent society is a personified metaphorical usage, meaning that the elements in society are no longer merely human intelligent entities but include an increasing number of machine intelligent entities and elements that integrate the two [5]. When various problems and changes arise in society, machine intelligence entities can collect all kinds of data and information through technical means, respond based on in-depth data mining, and constantly receive feedback to adjust their behavior. It is even possible to make predictions and take preventive measures before problems occur. This represents a leap from quantitative change to qualitative change compared with the sluggish response in traditional society.

The essence of the intelligent society is a complex system with increasingly strong coupling of "cyber, physical, and social system" (CPSS), that is, the integration of the physical world with human society, the integration of the real world with the virtual world, and the continuous improvement of the level of human–machine fusion intelligence [6]. As shown in Figure 1.4, the operating logic of CPSS includes three parts. (1) Physical space: various online or offline resources (applications, platforms, data, algorithms, and facilities) in the physical space are virtualized and released in the form of services. (2) Cyberspace: supporting intelligent data processing for informed decision-making, which can not only create "virtual organizations" in various fields (e.g., families, enterprises, and governments) but also define the workflow of various public affairs (e.g., smart government affairs, smart transportation, and smart security). (3) Social space: involving the coordination of interests among the government, enterprises, and citizens, to achieve value creation and circulation between demanders, suppliers, and service operators. Table 1.1 summarizes the current status of the intelligent society according to the three development stages, including both the advantages of intelligent technology in dealing with various social governance issues and the potential risks of intelligent technology when confronted with complexity.

In order to achieve this goal, intelligent social governance requires consideration from two aspects: on the one hand, the emergence of intelligent society is a bottom-up, self-organizing, and self-growing emergence process, and the overall state of the system depends on the spontaneous interaction between different intelligent subjects; on the other hand, intelligent society is also a product of top-down planning, and the laws obtained by big data analysis can be used to change the design and evolution path of the social ecology. Although a lot of progress has been made in the research of intelligent social governance, it still faces a series of problems and challenges caused by complexity [14]. It is necessary to complete the transformation from "comprehensive coordination" to "game evolution," from

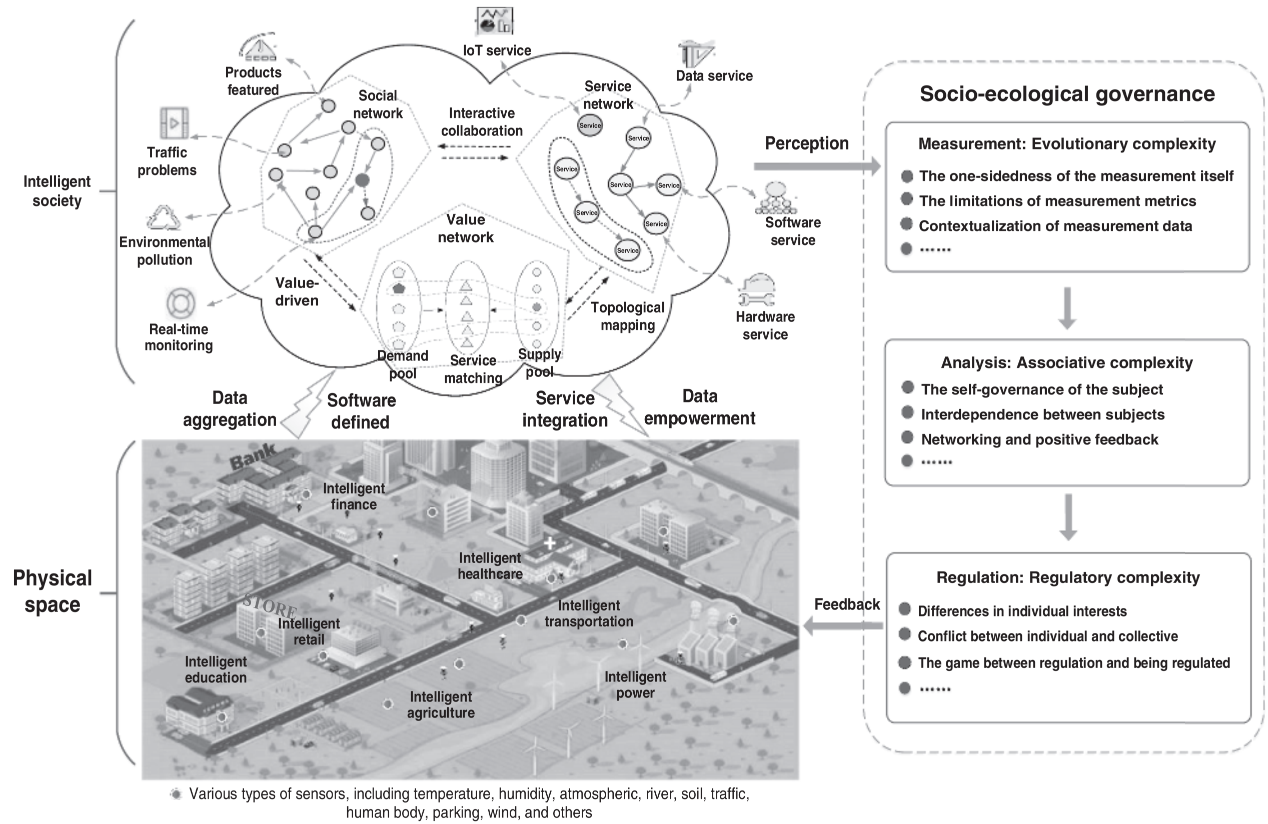

Figure 1.4 Intelligent society with CPSS characteristics.

Table 1.1 Successful Application and Potential Threats in the Intelligent Society.

Application Scenario	Successful Applications	Potential Hidden Dangers
Phase 1 (1998–2012) Internet Intelligence	Machine intelligence mainly stays in the Internet world. In response to the information overload problem in the Internet era, an information intermediary platform is built between suppliers and demanders to provide accurate recommendations for users. Representatives in the e-commerce field include Amazon, Taobao, etc.; representatives in the information field include Google, Netflix, Toutiao, etc.	Technology: Users may suffer from information cocoons [7], algorithmic discrimination [8], etc.; algorithmic drift may also lead to inaccurate predictions [9, 10]. Society: The centralization of data leads to excessive power in a small number of platform companies, which poses a risk of manipulating users and exacerbates the wealth gap and conflicts between third-party suppliers and platforms [11].
Phase 2 (2011 to Present) The Physical World is Intelligent	Machine intelligence has begun to penetrate into the physical world. In the physical world, there is a common contradiction between limited service capabilities and high-speed growth demand. Traffic congestion, retail, energy shortages, and environmental pollution all reflect the lack of dynamic service capabilities and efficiency of infrastructure. Problems with public facilities such as finance, education, and medical care reflect the lack of public service layout, supply, and service quality. The goal of intelligence is to change the current supply–demand matching situation, or to eliminate the information asymmetry between supply and demand, or to significantly improve supply capacity. Typical representatives include Uber, Meituan, and Hema Fresh in O2O life services; Alipay and PayPal in financial services; Alphabet's "Sidewalk Toronto" project in smart cities, and Ali's city brain.	Technology: Machine intelligence mostly makes decisions based on historical circumstances and is powerless to respond to emergencies, such as the impact of a financial crisis on personal credit or the impact of a sudden outbreak on the scheduling of medical resources. Society: In many cases, smart cities hope to achieve optimal scheduling of supply and demand matching without increasing supply. However, local optimization in complex networks may not necessarily lead to global optimization. Whether the smart service system can really solve the problem remains in doubt. For example, smart navigation services may fail during peak hours due to big data traps because it will lead to a competition between a large number of users for the same road resources [12].

Phase 3 (2015 to Present) Autonomous Intelligence	Machine intelligence is gradually achieving autonomous decision-making and continuously driving the accelerated evolution of human society. Its characteristics are as follows. (1) Enhanced integration: All human, material, and environmental factors are incorporated into the intelligent network and are fully perceived, recognized, and calculated. (2) Comprehensive intelligence: Machine intelligence will be widely distributed in society and seamlessly integrated with human intelligence. (3) Detailed planning: While allowing for unknown risks, machine intelligence can effectively provide public service products.	Technology: Socioeconomic systems are all super-complex systems, with many internal layers, complex influencing factors, and intricate relationship networks. The larger the scope of the problem, the greater the complexity of the data associations, and the possible scenarios increase exponentially. Simple, unified, and average centralized interventions lack adaptability and are difficult to deal with uncertain and global problems. The failure to predict financial crises and stock market fluctuations is a classic case, the reason for which is the endless emergence of various black swan events [13]. Society: There is a contradiction between the macro-control of the social and economic system and the autonomous behavior of individuals. Both sides are always in an evolutionary game, and it is difficult to have effective measures from beginning to end, such as urban planning and social ethical conflicts.

"macro description" to "causal analysis," and from "single indicator" to "value coordination," as specifically manifested in the following three aspects.

1.1.2.1 Evolutionary Complexity (Difficult to Measure)

The subjects in the social ecology not only are people with autonomous consciousness and strategic behavior but also gradually include various intelligent machines, human–machine fusion systems, social organizations, and digital platform companies. The AI system with increasing capabilities and the people and organizations empowered by AI are both autonomous and passive, both conflicting and cooperative, forming an evolutionary system of multi-agent game. As the number of collaborating subjects continues to increase, the dynamic interactions between the subjects become increasingly complex, and the probability of random deviations will increase. In addition, the transparency of the service process itself is very low, and the visibility of risks is easily obscured by various links and will eventually accumulate until they erupt. Without an appropriate performance measurement system (the comprehensive ability to do the right thing in the right way) to explicitly identify the risks in the service process, it is impossible to continuously improve and govern the social system.

1.1.2.2 Association Complexity (Difficult to Analyze)

The evolutionary complexity of social–ecological systems is essentially the organization and evolution from multi-subject behaviors and their associated service networks toward overall functions. With the accessibility and ubiquity of information technology, the associations and autonomous evolutionary behaviors among various subjects are constantly increasing, which often leads to unexpected emergent phenomena. Any governance strategy, through networked connections and positive feedback amplification, may quickly be associated with other events to produce a cascading "$1+1>2$" emergence, and even trigger "polarization" or "butterfly effect," which spills over into systemic risks. However, most of the current analytical methods focus on "description" rather than "explanation." They can present the evolutionary process, but it is difficult to provide insightful causal analysis to understand how the system operates.

1.1.2.3 Regulatory Complexity (Difficulty in Regulation)

As far as the social–ecological system is concerned, different individuals have different interests and needs. Sometimes, individual interests are inconsistent with the overall interests of the system, and there may even be conflicts. In addition, its internal subjects are diverse, including not only people and institutions but also AI algorithm-based platforms. They all have autonomous consciousness and learning ability and will change as the external environment changes. There is a two-way feedback mechanism between the social system and the individual behavior, which will cause the system to produce complex second-order emergence. Therefore, there will often be “a situation where subordinates find ways to circumvent superior policies,” which will greatly reduce the effectiveness of strategy implementation. This requires that the governance strategy should not only consider individuals’ pursuit of interests to ensure the motivation and vitality of system development but also resolutely prevent the interest imbalances and avoid threatening the order and stability of the system. These have posed challenges to the existing social–ecological governance capabilities.

1.1.3 The Rise of Computational Social Science

In order to model, analyze, design, and manage complex social systems, we need to shift through the myriad and complex phenomena to find unique perspectives for observing and understanding the intelligent society. Against this background, in February 2009, 15 top scholars from world-class universities such as Harvard University and MIT jointly published a paper “The Advent of the Era of Computational Social Sciences” in *Science* [15]. In 2012, 14 famous European and American scholars jointly issued a “Declaration on Computational Social Sciences,” and the voice of *Computational Social Sciences* overshadowed other terms [16]. In 2020, these scholars once again published a joint paper in the journal *Science*, highlighting the problems and challenges faced by the development of computational social sciences [17]. In the development of computational social science, many subdisciplines and subfields, such as computational economics [18], computational finance [19], computational histology [20], and computational epidemiology [21], have evolved.

Researchers in computational social science come from both the social sciences and computational sciences. Traditionally, social scientists have prioritized providing satisfactory explanations for the behavior of social systems, often relying on causal mechanisms in substantive theories. In contrast, computer scientists have traditionally focused on developing accurate predictive models, regardless of whether these models fit causal mechanisms or even whether they can provide explanations. Therefore, the standard practice for social scientists is to fit their models entirely “in sample” because they try to explain social processes rather than predict outcomes, while for computer scientists, evaluation using “out-of-sample” data is necessary. In addition, computer scientists typically allow the complexity of the model to increase as long as it continues to improve predictive performance, while for social scientists, the model should be based on substantive theory and is, therefore, constrained by substantive theory [22].

Both approaches are valid under their respective conditions, and both have produced a large number of fruitful scientific results. However, both approaches have also been criticized: on the one hand, theory-driven empirical social sciences have

Whether intervene / Whether predict	No intervention or allocation changes	Under intervention or allocation changes
Focus on specific features or effects	Quadrant 1: Descriptive modeling describes past or current situations (Basic activities, such as statistical surveys network community detection)	Quadrant 2: Explanatory modeling estimates the impact of changes (Social sciences, such as field experiments)
Focus on predicting outcomes	Quadrant 3: Predictive modeling predicts outcomes for similar future situations (Intelligent sciences, such as recommendation algorithms)	Quadrant 4: Integrative modeling predicts outcomes and estimates the impact of unseen situations (Intelligent sciences + Social sciences) ?

Figure 1.5 Classification of research methods in computational social science.

been criticized for being unable to predict results of interest and unable to provide solutions to real-world problems; on the other hand, the predictive models given by computational science have been criticized for being nongeneralizable, inexplicable, and biased. In order to promote the development of computational social science, we need to incorporate the thinking and methodologies of these two classical traditions, while also reconciling the different cognitive values of social science and computational science to produce new methods that both sides can agree on. Figure 1.5 shows four quadrants, each describing the main research methods of computational social science.

Descriptive modeling (quadrant 1) involves thinking about, defining, measuring, collecting, and describing relationships between quantities of interest. Activities in this quadrant include traditional statistical and survey research, as well as computational methods such as topic modeling and community detection in networks. Much of what we know about public opinion, economic conditions, and everyday life experiences comes from survey research. For example, recent studies have documented significant differences in mortality rates, wealth gaps, and intergenerational economic mobility among racial and ethnic groups. Qualitative and comparative methods popular in sociology, communication, and anthropology also belong to this quadrant. To date, most of the progress in computational social science has been made in using digital signals and Internet platforms to study concepts that were previously unmeasurable. In other words, descriptive work, both qualitative and quantitative, is useful and interesting in its own right and is also fundamental to activities in the other three quadrants.

Explanatory modeling (quadrant 2) refers to activities aimed at identifying and estimating causal relationships but are not directly concerned with predicting outcomes. Most traditional empirical sociology, political science, economics, and psychology fall into this quadrant, including statistical modeling of observational data, laboratory experiments, field experiments, and qualitative methods. Some methods (e.g., randomized or natural experiments) isolate causal effects by design, while other methods (e.g., regression modeling, qualitative methods) invoke causal explanations based on theory. Methods in this quadrant tend to prioritize simplicity, considering only one or a few characteristics that may affect the outcome of interest. These methods are very useful for understanding individual causal relationships, forming theoretical models, and even guiding policy. For example, social experiments show that job applicants with “black” names are less likely to get interviews than those with “white” names. This reveals the existence of structural racism and can inspire specific policy interventions.

Predictive modeling (quadrant 3) refers to activities that attempt to directly predict outcomes of interest but do not explicitly focus on identifying causal relationships. “Predictions” in this quadrant may or may not be about actual future events; however, in contrast to quadrants 1 and 2, they refer specifically to “out-of-sample” predictions, meaning that the data on which the model is evaluated (the test data) is different from the data on which the model is estimated (the training data). Activities in this quadrant include time series modeling, forecasting competitions, and many supervised machine learning activities, ranging from simple linear regression to complex deep neural networks. From a policy perspective, it is helpful to have high-quality predictions about future events, even if these predictions are not causal in nature. For example, applications of machine learning abound in Internet advertising and recommender systems. Although these algorithms cannot determine what caused people to click or content to go viral, they can still provide useful inputs to policymakers. That said, there is often an implicit assumption that the data used to train and test the model comes from the same data-generating process, akin to making predictions in a static (albeit potentially noisy) world. Thus, while these methods are generally applicable to fixed data distributions, they may not be applicable to settings where features or inputs are actively manipulated (such as in controlled experiments or policy changes).

Integrative modeling (quadrant 4) refers to activities that attempt to predict as-yet unseen outcomes based on causal relationships. More specifically, quadrant 3 focuses on data that are out-of-sample but still come from the same (statistical) distribution, and the focus here is on generalizing “out-of-distribution” to scenarios that may vary naturally. This category includes changes in the distribution that we have observed before as well as completely new and more extreme situations (due to some uncontrollable factors, or due to some deliberate intervention, such as an experiment or policy change). Integrative modeling, therefore, requires focusing on estimating causal effects (quadrant 2) rather than simply associative effects and considering the impact of all these effects simultaneously to predict outcomes as accurately as possible (quadrant 3). Ideally, work in this quadrant will give high-quality predictions of future outcomes in a (potentially) changing world. Research in this quadrant is relatively rare and more challenging.

1.2 Methodological Framework of Computational Experiments

1.2.1 Computational Experiment = Agent Based Modeling (ABM) + Experiment

In response to the challenges faced by ABM in the field of causal inference, Professor Fei-Yue Wang systematically proposed the basic ideas, concepts, and methods of computational experiments in 2004, emphasizing the circular feedback relationship between artificial systems and actual systems [23, 24]. Computational experiment method is an improved and extended version of ABM. ABM is not simply used as a simulation tool but as an "artificial social laboratory" that "spontaneously grows and cultivates" an alternative version of the actual system and can conduct various "counterfactual experiments" on system behavior and decision analysis. On the one hand, computational experiments use ABM to emphasize vertical causality, pay attention to the causes and formation process of phenomena, and give causal significance to the cross-level correlation information generated by ABM (the connection between micro-mechanisms and macro-emergence). On the other hand, computational experiments "use counterfactual algorithms to construct multiple worlds" to emphasize horizontal causality, establish a probabilistic relationship between model parameters and macro-emergence through experimental mechanisms, reveal the patterns and laws within the system, and provide "description," "prediction," and "prescription" for the possible operation of the actual system. Because the virtual foundation on which the experimental mechanism is based, that is, the attributes, behaviors, and local environment of the agent, is a replica of its real-world counterpart. Therefore, the probabilistic relationships established between different levels of analysis can be viewed as counterfactual connections across levels of analysis in the real world.

Computational experiments belong to the research path of "generative explanation," that is, to trace the causes by exploring the mechanisms that can show how social phenomena arise [25]. Traditional inductive interpretation uses statistical methods to derive general rules from data, and these rules are used to process data and are independent of data. However, generative explanations are based on the use of micro-interaction rules to derive macroscopic emergent structures, that is, general laws necessarily depend on the basis on which they are generated. Thus, generative explanations methodologically offer the idea that "how we know" is the basis of "whether we know," a connection that is precisely what inductive and deductive methods lack. Generative explanations are different from traditional deductive or inductive paths and place individual differences, local interactions, and the evolution of rules, which are ignored by traditional equilibrium analysis, at the core of the discussion. As shown in Figure 1.6, the computational experiment method is an "experiment + deduction" mechanism to explore the dynamic patterns, which consists of the following four core steps.

1.2.1.1 Preparation

The first step in a computational experiment is preparation, and the artificial society model can only be used for the computational experiment if it is proven to be consistent with the actual scenario. In the process of research, the artificial society model needs to be continuously adjusted, and occurred situations can be used as a benchmark for model adjustment, similar to the standard sample in chemical experiments, until the simulated situation and the real situation match in terms of statistical distribution characteristics. In order to explore as many unknown scenarios as possible in the real world, it is necessary to analyze the conditions under which these unknown scenarios occur and the likelihood of these conditions, including (1) an appropriate number of agents, with neither all agents nor some key agents ignored; (2) clear boundaries, abstracting the random perturbation factors that affect the state and properties of the system into boundaries, and eliminating the rest of the irrelevant parts; (3) agent–agent, agent–environment, and environment–environment interactions are based on knowledge rather than data, i.e., those linear/nonlinear, deterministic/random, static/dynamic function descriptions are based on the abstract relationship of facts; and (4) eigenvectors are set up to represent the state of the system based on the research objectives, and these variables will be combined according to a certain relationship to achieve a measurement of the state of the system.

1.2.1.2 Design of Experiments

Computational experiments take the "multi-world" view of complex systems research, where the results of the experiment are treated as a possible "reality" that behaves "differently" but "equivalently" from reality. Experimental design follows an experimental methodology, including the setting of initial rules and the testing and selection of models, either to reproduce some real-world settings or phenomena or to construct and observe possible worlds. Generative experiments deal with multivariate realizable cases: what if multiple microscopic mechanisms generate macroscopic patterns P (or rules) to be explained? The role of "experiments" is to assess the sufficiency of the generation of microscopic mechanisms: if multiple microscopic mechanisms can derive P, they can only be used as candidate explanations, and the most reliable explanation needs to be determined at the microscopic level. Therefore, it is necessary to continuously

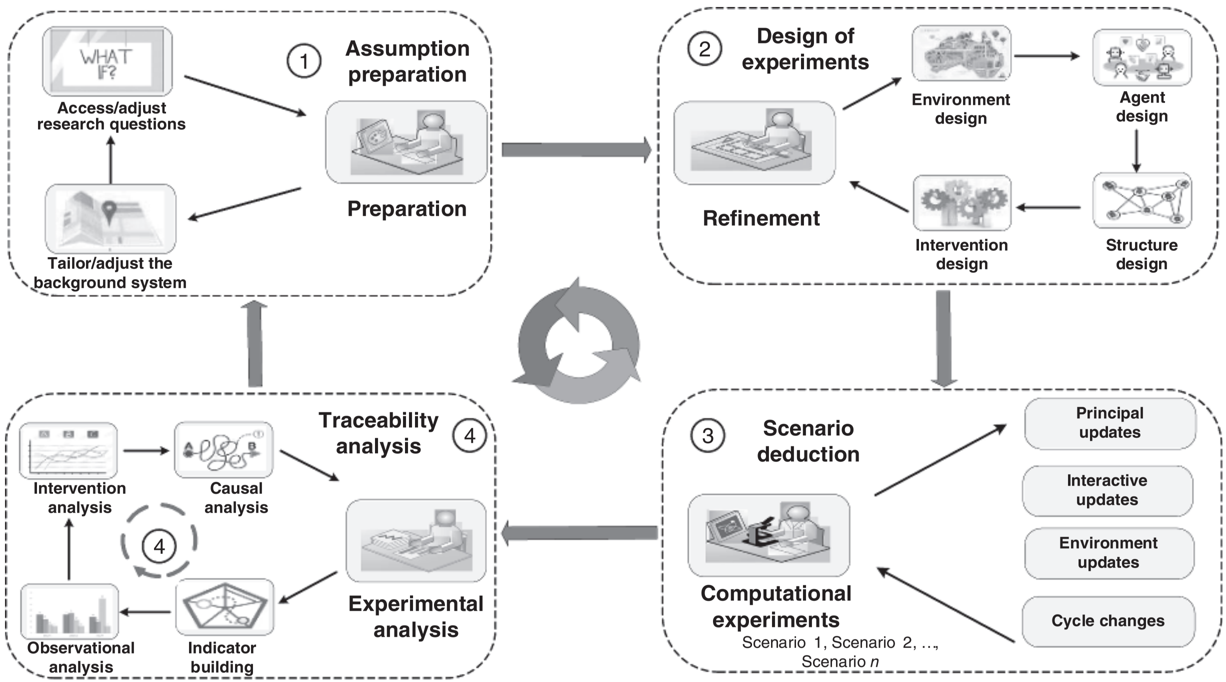

Figure 1.6 The process model of the computational experiment method.

deduce according to the experimental design scheme, and the whole tracing process is a process of continuous experimentation. Further, the same initial setup may evolve into different possible outcomes. By designing counterfactual scenarios that have never happened in reality, it is possible to identify potential adverse effects that may occur and provide "references," "predictions," and "guidance" for possible scenarios.

1.2.1.3 Scenario Deduction

Computational experiment scheme deduction is deductive, which refers to the computational process of deriving macro rules from the initial configuration of the agents. ABM is particularly suitable for generative inference, which is to convert the generation process into an agent-based computational model and reveal the micro-level generation mechanism of macroscopic rules through computational simulation. In this process, the ability to generate the macroscopic results of interest is key. Because each agent model is a computational program, its running process can be expressed by a loop function. Assuming the n-th state of the system, then the $(n+1)$ state is deduced in a strictly deductive and computational manner. From the initial setup of the agents to every subsequent step, the computer implementation can be equated with the deduction of theorems. If x is considered the initial state of a set of agents, then it can be updated repeatedly according to the local interaction rules: if x, then y.

1.2.1.4 Traceability Analysis

From the perspective of mechanism, the correlation and continuous covariation between social phenomena and variables cannot explain social phenomena but need to be explained by a series of agents and their behaviors that cause phenomenal changes. Mechanisms can help us understand why a particular cause is of explanatory relevance. Something like: "Surprising fact C has been observed; if A is true, C is certainly true as well; therefore, there is reason to guess that A is true." Here, hypothesis A is an attempted guess, and whether or not it can be recognized depends on A being able to explain phenomenon C. So, the slogan of generative social science is: if you can't generate it, you can't explain its emergence. In other words, the emergence of macroscopic outcomes depends on the micro-mechanism of local interactions, and this sufficiency of generation is a necessary condition for explaining how macroscopic outcomes are generated.

1.2.2 Computational Experiments + Emerging Technologies

In the field of social simulation, customized methods and solutions are the norm, and the lack of a unified methodological framework limits the use of computational experiment methods by many interdisciplinary researchers. The individual steps of computational experiments are the vehicles through which emerging technologies come into play [26]. In recent years, various intelligent technologies, such as reinforcement learning, digital twins, large language models, and causal inference, have had a considerable impact on computational experiment methods. The following are some of the interdisciplinary research studies carried out by computational experiments and various intelligent technologies:

1.2.2.1 Computational Experiments + Machine Learning

When dealing with a large number of individual agents with different behaviors, it is not easy to design the decision rules for each agent. Generally speaking, we assign some simple deductive rules to each agent to govern their decision-making process, and the resulting macroscopic phenomenon is called emergence. However, it is generally accepted that such models are often not fully representative of the true way individuals make decisions on behavior. There are a variety of factors that affect decision-making, including the complex internal state of the agent, the agent's understanding of the environment in which it operates, and the corresponding dynamic rewards and risks. For human society, there may also be complex social factors, different knowledge bases, and agent learning curves [27]. Therefore, the necessity of combining learning logic, uncertainty, and induction has received increasing attention in the field of intelligence, and related technologies include knowledge discovery and representation, uncertainty reasoning, and machine learning [28]. ABM's developers have been facing difficulties in designing behavioral rules for agents. By employing machine learning techniques, traditional agent behavior rules can be transformed from hard-coded rules into adaptive models [29]. Although there is a lot of research on applying machine learning to ABM, the universally applicable scenarios, frameworks, and implementation processes have not been well addressed. Among them, representative works include Ref. [30], which introduces the application of machine learning techniques based on classification and regression in ABM, and Ref. [31], which focuses on the application of reinforcement learning to ABM.

1.2.2.2 Computational Experiments + Large Language Models

In an artificial society, the ideal model for an agent is an autonomous agent, capable of running in a loop in its simplest form, with each iteration generating self-directed instructions and actions. They do not rely on humans to direct conversations and are highly scalable. In the past, academia focused on how reinforcement learning could be used to improve AI agents. The emergence of large language models has undoubtedly brought new possibilities to the development of AI agents. In 2023, AI agents ushered in a big explosion, and multiple AI agents such as BabyAGI and AutoGPT sprang up like mushrooms after a rain. One of the most intriguing projects is the "virtual town" built by Stanford researchers, where 25 AI agents survive and can not only engage in complex behaviors (such as throwing a Valentine's Day party) but also demonstrating human-like social behaviors [32]. In social simulation, the key to using large language model agents is their excellent role-playing ability, which is essential for realistically portraying various characters and perspectives in reality. Research in this field is growing rapidly, encompassing a variety of fields such as social sciences, games, psychology, economics, and policymaking [33–36]. In the future, AI agents may not be individual entities, but many AI agent organizations, and even an AI agent civilization, will emerge. How to combine large language models with computational experiments is still in the stage of experimentation and exploration, and various technical challenges need to be faced [37].

1.2.2.3 Computational Experiments + Social Networks

The evolution of complex social systems is determined not by individual behavior but also by the behavior of complex networks embedded in individual relationships, communities, and markets. In order to understand these complex social processes, researchers must focus on the dynamic interaction of individual behaviors and social network structures. Social network analysis (SNA) rigorously quantifies the patterns of relationships between social entities through a formally defined graph theory approach, which can be used to understand various social phenomena [38]. ABM has also proven to be a valuable method for solving complex tasks in analyzing interactions between individuals or groups. Since the interaction between agents can be mapped as nodes and links in network science, the combination of the two approaches is easy to achieve. Embedding the network into the ABM makes the interaction between agents no longer limited to spatial relationships but also through social networks, which provides new opportunities to gain insight into the behavior of social systems. The integration of social networks into computational experiments can help understand these processes [39]. In addition, ABM can supplement the sampling bias of network structure that is common in empirical methods in social science. Since there is little complete network data available, it is often not possible to get a complete picture of all node relationships. Computational experiments can be used as "virtual laboratories" to explore networks in space and time and to test hypotheses about causality [40]. Therefore, the combination of computational experiment method and network analysis methods can help bridge the gap between the two types of methods (theoretical and empirical), opening up many research possibilities. Many interesting examples demonstrate this potential, such as epidemiology, marketing, or social dynamics.

1.2.2.4 Computational Experiment + Experimental Design

For social simulation, each scenario is multi-node and nonlinear, and each AI agent has N choices at any node, resulting in countless storylines. As the complexity of the system increases, the number of influencing factors increases exponentially. Moreover, there are also human and social factors, not only randomness but also human initiative, which leads to greater complexity. Each experiment will have different influencing factors and different research objects, so the core of the whole experiment lies in the experimental design, and it is necessary to determine the experimental objects, experimental objectives, influencing factors, and intervention methods. For example, whether the experiment focuses on variance or treatment effects, whether the experimental population is homogeneous or heterogeneous, or whether the factors of the experiment are single or multifactorial. These differences mean that traditional experimental design (design of experiments [DOE]) approaches may not adequately address the problems faced by computational experiments [41]. If we cannot identify appropriate response variables and influencing factors, we will not be able to explicate these emergence processes, let alone continuously improve and govern complex social systems. Compared with traditional simulation design, the experimental elements emphasized in computational experiments are not limited to the value of a certain variable, but may involve different data structures, and are difficult to quantify, which is a challenging problem at present.

1.2.2.5 Computational Experiment + Causal Inference

An interesting feature of computational experiments is that "the patterns, structures, and behaviors that emerge from the model are not the result of explicit programming but are generated through the interaction of agents." Sensitivity analysis techniques are commonly used to determine the effect of changes in input parameters on the output variables of artificial society models [42]. However, sensitivity analysis does not elucidate causal relationships between different elements in the model. These causal relationships are essential for a proper understanding of the emergent properties of the modeled system. In order to analyze causality, the field of causal inference has been pioneered by Rubin [43] and Pearl [44]. The focus in this area is on the construction and analysis of so-called cause–effect diagrams, such as directed acyclic graphs (DAGs). By encoding the causal structure between different variables, these diagrams can be used to analyze the (causal) independence of variables, as well as the causal paths between variables. In computational experiments, there are two advantages to using causal findings to analyze systemic emergences [45]. First, it provides researchers with an alternative way to understand the emergent properties of artificial society models and the real-world systems they mimic; it also provides insight into what factors lead to the emergent behavior of the model. This can lead to potentially unforeseen explanations for emergent attributes that cannot be revealed by sensitivity analysis or machine learning techniques alone. Second, the causal diagram provides a clear representation of the underlying mechanisms in the artificial society model. This allows the modeler to effectively communicate the results externally to nontechnical audiences. However, research in this area is still in its infancy.

1.2.3 Computational Experiments + Applications

With the help of computational experiments, researchers can expand their research scope to the intersection of social science and intelligent science from their own disciplinary standpoint and can start from a "problem-oriented" approach, cooperate with experts in other fields to study many interesting and novel topics, and deal with highly characteristic social big data. At present, computational experiment methods have shown great application prospects in many social fields, especially in many important fields related to the management and regulation of complex systems, such as social governance, public health, and financial markets. The following are some of the interdisciplinary research efforts carried out by computational experiments with various social scenarios:

1.2.3.1 Computational Experiments + Public Health

Computational epidemiology is a multidisciplinary field that aims to use computers to understand and control the spatial spread of diseases (e.g., SARS, H1N1, and COVID-19) in populations. Traditional forecasting models rely on a large number of variable choices and differences in knowledge, attempting to make the best estimates with uncertain information. However, the epidemic spread is a dynamic and uncertain process, which has not only many influencing factors but also many unknown areas and emergencies, which makes it extremely difficult to predict and research. At present, computational experiments have become an important method to study the large-scale spread of infectious diseases and are mainly used to predict the spread trend, pre-assess the impact, and optimize intervention strategies [46]. However, there is no computational model that is completely consistent with the real physical propagation process, and all models are only approximate abstractions of the actual propagation process. It is necessary to continuously reduce and avoid the influence of uncertainty from the aspects of data, model, computation, and result analysis, so as to obtain simulation results that are closer and closer to the real propagation process.

1.2.3.2 Computational Experiments + Economics

Computational economics is a branch of economics that uses computers as tools to study human and socioeconomic behaviors. Computational economics mainly uses computational experiment methods to find analytical and statistical solutions to complex economic problems. In recent years, complex economics has become a popular research direction, specializing in the study of the overall economic process as a dynamic system of interaction between agents, so it is a way of studying economic adaptation from the perspective of complex adaptive systems. Tesfatsion and Judd provide a comprehensive introduction to agent-based computational economics methods and their applications in various economic fields [18]. In 2021, Salesforce presented a new study called “The AI Economist” that proposes a two-layer reinforcement learning method based on economic simulation to discover tax strategies that can efficiently find a balance between economic equality and productivity [47]. Tilbury reviewed the historical obstacles faced by classical ABM in economic modeling [48].

1.2.3.3 Computational Experiments + Sociology

Digital technology is being fully integrated into human society with new ideas, new business forms, and models, exerting an extensive and profound impact on our production and life. On the one hand, social forces and market entities have participated in social governance more extensively with the help of digital networks and platforms, and governance entities have become more diversified. On the other hand, the transformation of social behavior in the digital era has had an impact on the traditional hierarchical regulation, and the governance model and means urgently need to be modernized. At the same time, civic awareness is constantly rising, the demands of social subjects are becoming more complex, and the governance goals are diversified. This poses new challenges to the unified regulation of diversity and consistency in the digital social system and brings higher requirements for the fairness and efficiency of social governance [49]. Computational experiments play a crucial role in the study of intelligent social governance, relying on the advantages of precision, controllability, ease of operation, and repeatability, which can simulate how the interaction between individual behavior and algorithmic behavior produces the overall social macro law and help us understand the role of information in the operation of the social system, such as social phenomena like information cocoons, platform monopolies, and algorithmic discrimination [50].

1.2.3.4 Computational Experiments + Political Science

Political theory, electoral mechanisms, geopolitics, and international relations have always been hot research directions in the field of political science. With the rise of technologies such as social media, recommendation algorithms, and intelligent assistants, people’s decision-making may be invisibly manipulated and directed toward interest-concentrated areas through various forms of algorithmic incentives. According to a recent study [51], when the proportion of people in a society exceeds a threshold, group selection is not necessarily optimal. The so-called “autonomous” behavior, which is constantly induced, is challenging the democratic foundations of social choice. Internationally, strategic game deduction is a very complex problem, involving many roles, and the influencing factors of each role's decision-making are also very complex. They will evolve over time, with challenges such as revenue ambiguity, diversity of strategies, and uncertainty of behavior. Computational experiments can deduce, analyze, and predict various political phenomena under various hypothetical pressures or extreme scenarios, such as the spread of political tendencies in social media, opinion conflict games and election predictions, and international strategic game deduction [52].

1.2.3.5 Computational Experiments + Finance

The complexity and inherent speculative nature of financial markets determine that they are often in a state of unbalanced fluctuations, and the implementation effect of financial regulatory policies is, therefore, facing great uncertainty. The financial market is a complex adaptive system, which is linked by a large number of parallel and interactive adaptive agents through economic behavior. Each agent can only obtain partial information of the whole system, but the agent has "adaptability" and can continuously learn and change its investment strategy through adapting to the environment. In 1987, Arthur et al. of the SFI research group constructed an artificial stock market that used a multi-agent model to explore financial market issues such as asset pricing, investor behavior, and market volatility. This model is a breakthrough achievement in the research process of agent-based financial market modeling, which pioneered agent-based computational finance (ACF) and became the real beginning of agent-based financial market modeling research [53]. Prof. Zhang Wei from Tianjin University has used computational experiments to study the possible financial market reactions of various regulatory measures and policies in depth, so as to evaluate the effect of policies and the feasibility of institutional construction [54].

1.3 Organizational Structure of the Book

As a research method that integrates social science and intelligence science, computational experiment methods integrate multiple disciplines such as economic science, computational science, complexity science, and intelligence science. Despite the efforts of researchers, computational experiment methods are not yet a mature set of tools, nor are they a complete set of theoretical systems, and there is still a huge gap between their prospects and practical applications. Therefore, in order to promote the research development of this field, this book will address the following three questions:

1) **How is it modeled?** The agent model is the core of computational experiments, and it also serves as the container for different intelligent knowledge to come into play. At present, most researchers manage the decision-making

process of each agent by assigning some simple deductive rules to them, resulting in macroscopic emergence. However, researchers generally agree that this model is often not fully representative of the real way in which social agents make decisions. A good agent model should have human-like characteristics, and there are various factors that affect its decision-making, including internal state, environment, and corresponding dynamic rewards and risks, and may even involve complex social factors, different cultural backgrounds, and the agent's learning curve. Therefore, how to use various AI technologies (such as large language models, reinforcement learning, and swarm intelligence) to improve agent model design (including heterogeneity, bounded rationality, learning evolution, and interaction) has become a key challenge for the sustainable development of this field.

2) **How to experiment?** In the computational experiment system, each scene is multi-node and nonlinear, and each AI agent has N choices on any node, resulting in countless story lines. As more agents are involved, the more diverse the agents are, the more complex the interactions will be, the number of influencing factors will increase exponentially, the probability of random deviation will also be greater, and the visibility of emergent phenomena will be easily overshadowed by various details. Researchers mostly focus on "description" rather than "experiment." They can deduce the evolution process of the system, but it is difficult for them to provide insightful causal analysis of emergent phenomena to understand the operation of the system and cannot give the laws behind the phenomena. Therefore, this book will focus on how to use computational experimental design to realize causal relationship mining and causal mechanism inference, so as to provide a decision-making basis for subsequent regulatory strategy optimization.
3) **How to develop?** As a multidisciplinary field, computational experiments involve a lot of domain knowledge. It is often difficult for researchers to clarify the relationship between AI technology and sand table models, between simulation and computational experiments, and between general settings and specific scenarios, and this dilemma is exacerbated by the emergence of various AI technologies. At present, most researchers focus on "explanation" rather than "prediction," and sand table deduction is relatively simple, which can often only be used to explain phenomena, but it is difficult to play the role of intelligent decision-making. In order to solve this problem, this book will focus on how to use a large language model technology to support the development of computational experiment methods, hoping to construct a suitable platform support for the implementation of computational experimental theories.

The organizational structure of the book is shown in Figure 1.7, which is mainly divided into four parts: basic theory, method framework, key technologies, and

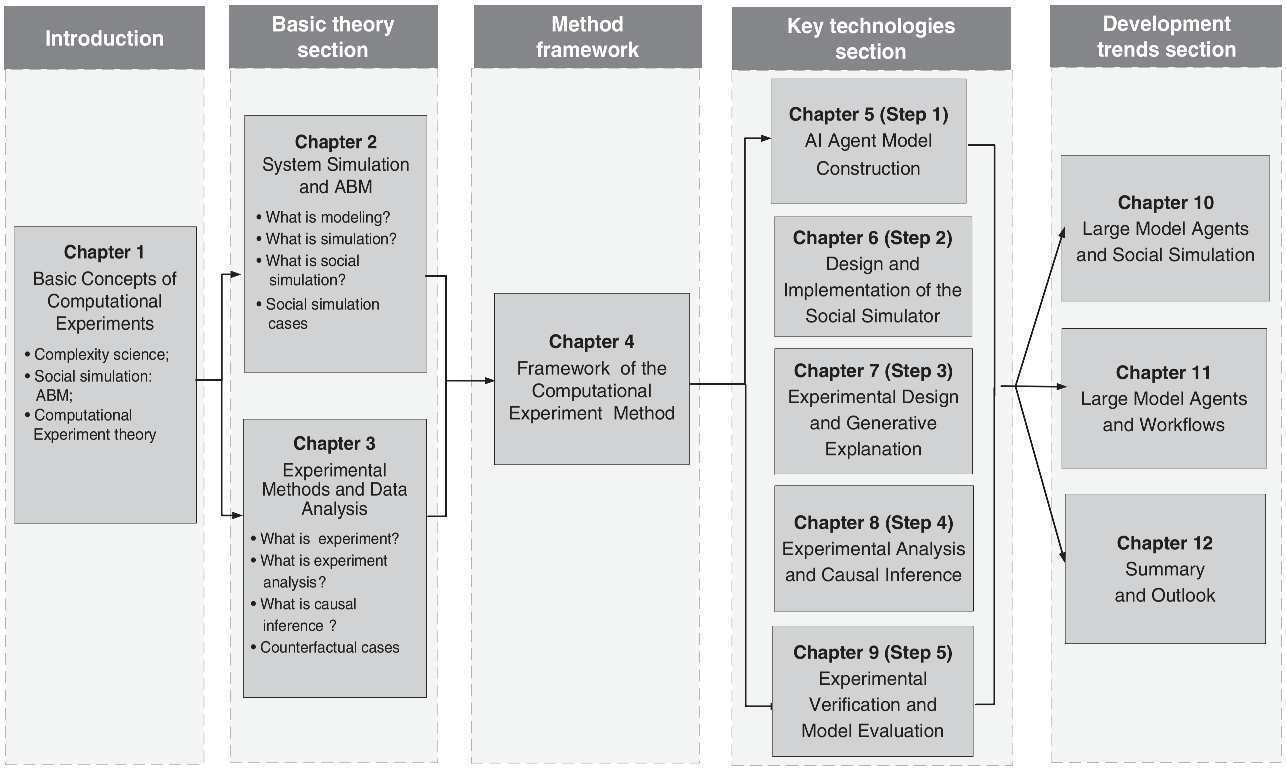

Figure 1.7 The structure of the content of the book.

development trends. The book adopts the research idea of "theory + practice," starting from the basic knowledge of computational experiments, so that readers can further analyze the experimental cases on the basis of understanding the theoretical models, so as to have a complete grasp of the computational experiment method. The details of each chapter are as follows.

1.3.1 Theory Section

This chapter mainly introduces the origin and ideological essence of computational experiment method and introduces the organizational structure and content of this book. This chapter sorts out the sources of complexity of social systems and thus leads to the research quadrant of computational social science. As an important tool in computational social science, ABM has made a lot of progress in many fields, but it also faces the dilemma of "causal inference." In this context, computational experiments provide a feasible way to analyze the behavior of complex systems and evaluate causal effects through the "ABM experiments." Finally, under the framework of computational experiment method, how to combine it with emerging technologies and application fields is introduced.

Chapter 2 mainly introduces the computational experiment method for physical systems. This chapter first starts from the concepts and examples of system simulation so that readers can understand the unique properties of computer simulation and the corresponding operating mechanism; then, it introduces the principles of system simulation and modeling to provide method guidance for the application of system simulation; finally, it introduces in detail the commonly used experimental design methods and statistical analysis methods of experimental data.

Chapter 3 elaborates on the computational experiment method for social systems in detail, which can provide some unique insights for the simulation and deduction of social complex systems. This chapter first introduces the development history, design principles, and causal challenges of ABM. Then, this chapter gives three basic models in social simulation: agent model, environment model, and rules model. Based on this, the concept of causal inference is introduced, especially counterfactual inference based on virtual scenes. Finally, the classic social simulation cases are given as follows: Sugarspace model, AppEco model, artificial stock market model, service bridge model, etc.

1.3.2 Framework Section

Chapter 4 introduces the computational experiment method framework, which consists of five parts: artificial society modeling, experimental system construction, experimental design, experimental analysis, and experimental verification. Then, the implementation platform of the method is given, which mainly includes four core parts. (1) Sand table design module: builds AI agent and AI society. (2) Computational experiment module: provides tools for governance experiment design and experimental operation analysis. (3) Simulation engine module: decouples the design of sand table scene construction from multi-agent operation management. (4) Scene docking module: is a hub that connects practical applications and sand table scenes and can use 2D scenes, GIS modeling, 3D scenes, etc. according to needs.

1.3.3 Technical Section

Chapter 5 focuses on the first step of the computational experimental method: artificial society modeling. The difficulty of social system modeling lies in the modeling of human characteristics, including heterogeneity, bounded rationality, learning evolution, and interaction. In view of these difficulties, this chapter introduces in detail the four levels of artificial society modeling framework: autonomous feature modeling of AI agent, evolutionary feature modeling of AI agent, interaction feature modeling of AI society, and emergent feature modeling of AI society. The model framework is customizable and can use a variety of popular intelligent technologies to provide support for the construction of computational experiment systems.

Chapter 6 focuses on the second step of computational experiment method: experimental system construction. This stage mainly solves two problems: (1) how to map a specific domain model to a general artificial society model, including the agent model, the environment model, and the rule model, and provides the corresponding model docking cases and (2) how to use the control flow to integrate many model components of the artificial society, mainly the integration of the agent model and the environment model, and make the whole artificial society operate dynamically through the system engine, so as to lay the foundation for the subsequent simulation and deduction.

Chapter 7 focuses on the third step of computational experiment method: computational experimental design. Traditional experimental design methods cannot solve the problems of randomness and initiative in social simulation. In order to address this challenge, this chapter proposes a framework for computational experimental design: (1) to determine the influencing factors and response variables of the system through descriptive modeling of the artificial society, (2) to describe deterministic and nondeterministic factorial experiment method through interpretive modeling of experimental design, and (3) to obtain a predictive meta-model that understands the dynamics of the system based on the data between the inputs and outputs of the artificial society. Finally, an automated scenario generation algorithm is proposed, and the effectiveness of the proposed method is illustrated by the case of API service market.

Chapter 8 focuses on the fourth step of the computational experiment method: computational experiment analysis. In view of the limitations of traditional analysis methods in explaining the behavior of social systems, this chapter proposes a causal inference framework for computational experiments, which mainly includes three levels. (1) Observational analysis: focusing on the possibility space modeling of the evolutionary path of social systems, identifying all the states that social systems may experience and the probability distributions of their occurrences. (2) Intervention analysis: Randomized controlled experiments are used as a means to observe how the change of the cause variable caused the change of the outcome variable, so as to mine the robust structural causal model between the variables. (3) Mechanism analysis: Using the evolution of the world model within the agent as a tool, we can understand how individuals at the micro level lead to the emergence of phenomena at the macro level by analyzing the agent's behavior trajectory and thinking chain.

Chapter 9 focuses on the fifth step of the computational experimental method: computational experimental validation. How to evaluate the accuracy and validity of computational models is a difficult problem, which hinders computational experiments from becoming a more powerful tool for studying the operation of complex systems. In order to address this challenge, this chapter introduces a comprehensive capability maturity assessment framework for computational experiments, which provides a comprehensive assessment in terms of expectations, theoretical basis, data sources, intermediate stages, and result realization and evaluates whether the model meets expectations by comparing expectations and implementations. Finally, this evaluation framework is used to analyze and evaluate several representative models of COVID-19 to help decision-makers identify more mature and valuable models and point out to modelers the direction in which the models can be improved in the future.

1.3.4 Trending Section

Chapter 10 introduces the convergence trend of large language model agents and social simulations. The biggest advantage of large language model agents is that simulation agents with human-like characteristics (context learning, continuous learning, inference, etc.) can be developed so that the constructed artificial society also exhibits similar characteristics to real social systems (organized cooperation, reasonable competition, information dissemination, and group emergence). Starting from "Stanford Smallville," this chapter first explains how to use a large language model technology to achieve a sandbox environment similar to "Sims," in which each agent has a different portrait and can communicate with each other to generate rich dialogue and behavior data. Then, under the guidance of the hierarchical modeling framework of artificial society (Chapter 5), the key feature implementation techniques of generative agent are summarized. Finally, a typical case of a large language model agent used in social simulation is given.

Chapter 11 describes the convergence trend of large language model agents and workflows. The autonomous agent uses large language models (LLMs) as a "powerful general-purpose problem solver" for more intelligent and automated problem-solving. Compared with a single agent, the multi-agent system can effectively simulate the cooperation mode of human group problem-solving, emphasizing diverse agent configurations and collaborative workflows between agents, so as to solve more dynamic and complex tasks. However, the division of labor and collaboration also brings communication costs and accumulated errors. This chapter focuses on the workflows, collaboration models, and technical challenges of autonomous agents to lay the groundwork for automating computational experiments.

Chapter 12 summarizes the content of the book and gives the focus of further research.

1.4 Chapter Summary

This chapter begins with the concept of complex systems, i.e., the reasons for the emergence of computational experiment method. Then, the ideas and application fields of computational experiment methods are introduced, and it is clearly pointed out that computational experiments are a higher level of computational simulation with the further development of computing technology and analysis methods, a feasible way to analyze the behavior of complex systems and evaluate the effects of various decisions, and an effective means to make up for the difficulty or even inability of traditional methods to experiment on complex systems. In addition, this chapter explains the organizational structure of the book and provides a guide for subsequent study of the book.

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