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2024 Nobel prizes in physics and chemistry: from neural network models to materials engineering

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2024 Nobel prizes in physics and chemistry: from neural network models to materials engineering

In this review, I will discuss the reasons for the 2024 Nobel Prize in Physics, the second neural network boom and its demise, which cannot be ignored, and the third neural network boom, backed by steady academic progress. In addition, I will discuss AI for Science, advocated by Demis Hassabis, winner of the Nobel Prize in Chemistry. The contributions of Japanese researchers whose work cannot be ignored will be described, and a new perspective will be presented on information creation, statistical mechanics, and data-driven science. AI for materials engineering, which is an extension of AI for science, is explained in terms of the 3+1 model of functional expression and the three levels of data-driven science proposed by our group.

Keywords

Neural network, Neuroscience, AI, AI for science, Data-driven science, AI for materials engineering

Subject classification codes: include these here if the journal requires them

1. Introduction

Artificial neural networks model the mechanisms of the brain by combining the neurons that make up the brain with the binary model of McCulloch and Pitts for neurons [1], which is similar to Ising spins. The Nobel Prize committee publicly stated that the 2024 Nobel Prize in Physics was for research on these neural networks, specifically its results in AI [2]. However, this research pertains not only to that but also to brain modeling, which falls under the scope of physics. This review describes the achievements of the 2024 Nobel Laureates in physics, Hopfield and Hinton, and their enormous ripple effects on physics, brain science, and beyond. AI will be discussed as a universal paradigm for application to all sciences, particularly materials engineering.

2. Research achievements and developments related to the prize

2-1. Research achievements

In 1982, Hopfield proposed a model of brain memory. The important point here is that the Hopfield model is similar to the study of magnets in physics, especially spin glasses. This led many physicists, especially statistical physicists, who had no connection to brain research, to enter the field of brain research, which led to great advances in theoretical research on the brain and had a major impact on brain science as a whole. The concept of attractor neural networks proposed by Hopfield became established in brain science, and experimentalists in the field began to conduct research based on this concept. Hinton made notable achievements in neural networks such as back-propagation and the Boltzmann machine in the mid-1980s [4, 5].

2-2. End of the second neural network boom and steady academic progress

Then, the second neural network boom, which Hinton himself helped to ignite, ended without producing the desired results. The central focus of AI and machine learning shifted away from neural networks and toward topics such as support vector machines and variational Bayesian methods. At a banquet during NeurIPS, the international flagship conference on machine learning, a side comment was made that mentioning the Hopfield model or back-propagation in a submitted paper was highly correlated with rejection, causing the attendees to laugh.

Even during this dark period following the second boom, research was steadily progressing. Hinton et al. explored various new learning machines, such as products of experts [6]. Amit et al. proposed a model based on the Hopfield model that describes properties of neurons in the temporal lobe of the higher visual cortex found by Miyashita's group [7, 8]. Matsumoto et al. proposed a model based on the Hopfield model that explains the neural dynamics of face-responsive cells in the temporal lobe responding to hierarchical images, as found by Sugase et al. [9, 10, 11, 12]. The temporal lobe is located far from the retina, which is where image information enters, and little is known about how this image information input at the retina is processed in the visual cortex up to the temporal lobe. Therefore, it is not possible to determine the purpose of the computation, which would require Marr’s three-level theory of computation [13]. In this context, an approach from the hardware level is essential, and the experimental findings of Miyashita’s and Sugase’s groups provided a basis for identifying the hardware that could be used to determine the purpose of the computation, which could be used to study the temporal lobe. Amit et al. and Matsumoto et al. used the Hopfield model to study the temporal lobe from the hardware level. Also important is the work of LeCun et al., who have dealt with MNIST and who were among the first to apply the error back-propagation method to the neocognitron architecture proposed by Fukushima, which will be discussed later [14, 15].

2-3. The third neural network boom

After this quiet period, neural network research began to break through the stagnation in the 2000s when Hinton et al. proposed using a two-layer circuit, the restricted Boltzmann machine, to pre-train each layer of a multilayer neural network, and showed that this framework could handle complex tasks [16]. In 2007, a symposium on neural network models was held at the post-conference of NeurIPS, and I remember a well-known Japanese machine learning researcher commenting that he thought the idea was a tall tale.

His impression was mistaken, and in 2012, Hinton’s team Super Vision entered the field of general object recognition and proposed Alex Net, a two-stage feature extraction + discriminator method that quickly overtook conventional methods [17]. Alex Net has led to the current flourishing of research in artificial intelligence. The remarkable performance of Alex Net garnered public recognition of the potential of multilayer neural networks, and the concept and field of deep learning thus finally emerged. This influenced various fields, and the gold standard of AI development was Google DeepMind's Alpha Go in 2016 [18]. AI with Alpha Go was able to beat humans at Go, which was considered far more difficult than chess or shogi, so the game is no longer a testbed for AI. By extension, games in general are no longer a testbed for AI. Hassabis, the head developer of Alpha Go, has proposed the paradigm "AI for science," saying that the next target of AI is science [19]. As per his declaration, Hassabis proposed Alpha Fold, which can predict the three-dimensional structure of proteins with astonishing accuracy [20]. It goes without saying that Alpha Fold has revolutionized the methodology of protein research. The module of deep learning called the transformer or attention mechanism, which was key to developing large language models and other models [17], can be understood as an improved version of the Hopfield model [22, 23].

The following is my personal opinion, but I believe that the main reason for this third neural network boom is not a fundamental change in theory but the speedup and spread of computers and the explosion of training samples via the Internet.

3. Contributions of Japanese researchers

We show here that the 2024 Nobel Prize in Physics is not based on the first-to-invent principle by introducing the pioneering work of Japanese researchers. The contents of this section are summarized in Figure 1. In 1972, Nakano proposed a prototype of the Hopfield model called the associatron [24]. Amari proposed an autocorrelated associative memory model equivalent to the Hopfield model in 1972, 10 years before the Hopfield model was proposed [25]. We should not forget that many Japanese researchers contributed greatly to the theoretical clarification of the Hopfield model [26-29]. Amari and Maginu proposed a statistical neurodynamics describing the macroscopic dynamics of recall in the Hopfield model [26]. The macroscopic dynamics of recall cannot be analyzed through the theoretical replica method for the equilibrium statistical mechanics of random systems proposed by Amit et al. [30]. Nishimori and Ozeki [27] used numerical simulations to verify the assumption of a Gaussian distribution of the crosstalk noise used by Amari and Maginu. As a result, they succeeded in showing numerically that the assumption of a Gaussian distribution holds when the early stage is successful. Shiino and Fukai developed a theory that treats the equilibrium state of the Hopfield model using a mean-field approximation of the statistical mechanics of random systems [28]. This theory is called self-consistent signal-to-noise analysis (SCSNA), and they showed that it can yield results equivalent to those of Amit et al. Many researchers noticed a numerical discrepancy between the results of the replica method and the theory of the stationary household limit of statistical neurodynamics, and they were eager to construct a theory to explain the difference. Okada noticed that Amari's and Maginu's statistical neurodynamics incorporated correlations of crosstalk noise at different times, and developed a theory to deal with these time correlations by extending Shiino's and Fukai's SCSNA [29]. This clarified the relationship between the equilibrium statistical dynamics of random systems and statistical neurodynamics, which significantly improved the theoretical understanding of the Hopfield model.

Amari proposed the error back-propagation method in 1969 [27], 19 years before Hinton did. However, this achievement by Amari is not specified in the Nobel Prize Committee report [2]. Fukushima proposed the neural network neocognitron on the basis of the experiments on the visual cortex of the brain by Hubel and Wiesel, who won the 1981 Nobel Prize in Medicine [4]. Fukushima proposed the origin of artificial intelligence research, which is now flourishing to the extent that it has become a social phenomenon. The neocognitron [8] is also a component of Alpha Go.

4. Ripple effects

4-1. Creation of statistical mechanical informatics and ddata-driven science

Kabashima of the University of Tokyo stated that Hopfield's greatest achievement was discovering and inventing the "field" of using physics in information science and engineering, including AI [32]. This field is called statistical mechanical informatics. Figure 2 shows a time line of the statistical mechanical informatics created by Okada [33] and further developed by Kabashima [32]. As shown in Figure 2, statistical mechanical informatics is a unique field that can handle a wide range of areas such as neural network theory, information theory, learning theory, and communication engineering.

In 1985, Amit et al. succeeded in theoretically deriving the storage capacity of the Hopfield model using the replica method developed in statistical physics of random spin systems [30], and Sourlas proposed the Sourlas code, an error-correcting code, with reference to the Hopfield model [34]. In 1999, Kabashima and Saad analyzed low-density parity check (LDPC) codes using the replica method and showed that LDPC decoding can be handled by the Thouless-Anderson-Palmer (TAP) method, which is a mean-field approximation for random spin systems [35, 36]. In 1988, Gardner used the replica method to derive the storage capacity of the perceptron [37], which Cover had derived using information-theoretic methods [38]. This trend spilled over into learning theory, and in 1990 Sompolinsky et al. derived the generalization error of the perceptron using a replica method [39]. In 2001, Tanaka derived the demodulation error of CDMA in telecommunications engineering using the replica method [40]. Tanaka and Okada showed that the demodulation dynamics of CDMA can be discussed in statistical neurodynamics on the basis of the mathematical similarity between the Hopfield model and CDMA demodulation [29, 41]. This trend has not stopped and has recently expanded into broader informatics areas such as mass testing [42], graph division [43], lossy compression [44, 45], the constraint satisfaction problem [46], optimization [47], matrix factorization [48], and bootstrapping [49].

To deepen and develop statistical mechanical informatics, the following projects were awarded by the Ministry of Education, Culture, Sports, Science and Technology's Grant-in-Aid for Scientific Research on Specific Areas: "Statistical Mechanical Approach to Probabilistic Information Processing" (Tanaka Kazuyuki, Assistant Professor, Tohoku University) from FY2002 to FY2005 [50], and "Deepening and Development of Statistical Mechanical Information" (Kabashima Yoshiyuki, Professor, Tokyo Institute of Technology) from FY2006 to FY2009 [51]. Furthermore, the subsequent project "Deepening Sparse Modeling and Creating High-Dimensional Data-Driven Science" (Masato Okada, Professor, University of Tokyo) was also selected by the Ministry of Education, Culture, Sports, Science and Technology's Grant-in-Aid for Scientific Research on Innovative Areas from FY2013 to FY2017 [52]. This project became a strategic goal of JST CREST/PRESTO [53], and it has become the core for data-driven science, which has flourished in recent years, to take root in Japan.

4-2. History of AI and AI for science

As shown in Figure 4, games have been used as a testbed for evaluating AI performance. In 1970, Winston introduced the program ARCH to learn concepts from examples in the world of building block play. In 1980, The Othello program Moor won one match against then World Champion

Hiroshi Inoue (1-5 in 6 games). In 1997, IBM's Deep Blue defeated world chess champion Garry Kimovich Kasparov in a series with two wins, one loss and three draws. This stemmed from a change in IBM's business model, whereby IBM decided to pursue profits from software rather than hardware. In 2011, IBM's computer Watson won a contest on the quiz show *Jeopardy* by defeating two previous champions. Finally, the gold standard for AI development came in 2016 with Google DeepMind's Alpha Go [14].

Alpha Go's head of development, Hassabis, presented the AI for science paradigm, saying that the next target for AI is science. True to his declaration, he proposed Alpha Fold, which can predict the three-dimensional structure of proteins with astonishing accuracy [16], leading to his winning the Nobel Prize in Chemistry in 2024. Hassabis stated, "What I'm really excited to use this kind of AI for is science, and advancing that faster. I was giving a talk at CERN a few months ago. I think it'd be cool if one day an AI was involved in finding a new particle" [15].

Here is an outlook on how AI for science will develop in the future. On the surface, AI for science is a paradigm that uses the advanced function approximation capabilities of multilayer neural networks in place of ordinary function approximators. Examples are AlexNet [8], Alpha Go [14], Alpha Fold [16], and the computation of physical quantities such as electronic states [54, 55]. The important point here is where the multilayer neural network is used in each sub-process of information processing. The function approximation ability of multilayer neural networks will continue to improve in the future, but what is more important is how these models are used. For example, Alpha Go uses a multi-layer neural network as a function approximator in reinforced learning. As for speech processing, a multilayer neural network replaces the hidden Markov model in the conventional framework of speech processing. There are fewer examples where end-to-end information processing from input to output is replaced by end-to-end information processing from input to output. In fact, as before, the key is how to design a modular structure that includes a multilayer neural network model.

Let us consider an example of this in the STEM field with the primary AI audience: AI for materials engineering. Figure 4 shows the 3+1 step model of functional expression proposed by our group [56]. Most of the modular configuration models of functional expression devised in materials engineering are in the category of 3+1 step models [57, 58]. Materials science and materials engineering have different objectives. Materials science studies the physical properties of materials, while the objective of materials engineering is to design materials with desired functions. More often than not, the function of a material is not determined solely from the physical properties of the material as determined by materials science. In some cases, such as the properties of the cathode or anode of a battery, the physical properties can be derived from first-principles calculations based on the compounds of the cathode or anode, but such cases are rarer. The function of a material cannot be deduced only from physics and chemistry.

Our group has therefore divided the process from matter to function into three steps, as shown in Figure 4. The left side represents the process of extracting the properties of matter. This process on the left is in line with physical models, and the properties of a substance are extracted using Bayesian inference and other methods. The right side represents the process of using the extracted properties as features to find their correlations with functions. This side cannot be described by a causal law like a physical law but is a module for predicting functions from features.

To guide the execution of these Bayesian inferences on the right and the data analysis with sparse modeling (SpM) on the left, we propose three levels of data-driven science [56]. These are proposed with reference to David Marr's three levels of data-driven science [13], which he discusses in the context of the three levels of understanding complex information processors: computational theory, representation and algorithms, and hardware implementation. He argues that it is necessary to integrate the three levels to understand complex information processors. Because experimental/measured data analysis is also a form of complex information processing, we need to refer to Marr's three levels. Therefore, we propose the three levels of data-driven science shown in Figure 5. The three levels are computational theory, modeling, and algorithms. At the computational theory level, the purpose of the data analysis and the strategy that enables the analysis are described in natural language. Next, at the modeling level, the computational theory is expressed in a mathematical model. Finally, an algorithm is devised to solve the mathematical model. Note that these three levels, as shown in Figure 5, are also used to solve simultaneous equations learned in eighth grade mathematics. Simultaneous equations are applied to seemingly completely unrelated problems such as the saltwater problem, where the purpose of data analysis and computational theory is to find the concentration and quantity of saltwater. This computational theory is implemented using a mathematical model called a simultaneous equation. This is at the level of modeling. Finally, simultaneous equations are solved with addition, subtraction, and substitution methods at the algorithmic level.

The similarity between data analysis and application of simultaneous equations is very important [59]. First, there is a reason why data analysis in different fields can be solved by the same algorithm. This also shows that the mathematical model that transforms and expresses the computational theory is independent of the target. Furthermore, because the mathematical model to be solved is independent of the target, it is clear that the algorithm to solve it is also independent of the target.

It is also clear that when learning data analysis, it is necessary to first concentrate on mastering the mathematical model and the algorithm for solving it, just as in the case of simultaneous equations. Once one is proficient in mathematical models and algorithms, one can derive the computational theory so that data analysis can be performed. From the above, if we follow the three levels of data-driven science, we can acquire the skills to perform universal data analysis regardless of the field.

SpM assumes that the features can be expressed in a linear function. Next, we examine all of the features to determine whether each is included in that linear function. If the number of features is p, the function is predicted by considering all 2^p-1 combinations, evaluating the cross-validation error and Bayesian free energy for each combination, and selecting the combination with the smallest values of both. Cover and Van Campenhout proved in 1977 that SpM requires this exponential-order computational complexity of features [60]. There are two approaches to this exponential-order computational complexity. One is called relaxation, an approach that transforms the problem into a more solvable problem. LASSO, proposed by Tibshirani in 1996, relaxes the problem from L0 optimization to L1 optimization [61]. Numerous other SpM approximation algorithms exist. Suppose that these SpM approximation algorithms are used to explore the mechanism of feature expression. In this case, the number of approximation algorithms may result in a different set of features to be selected, and this will not allow correct feature selection. Performing feature selection correctly requires rigorous calculations.

After the feature sets that provide the mechanism of function expression have been selected in this way, it is a matter of knowing how to change the process parameters of material production in the lower step of Figure 4 to appropriately control the selected feature sets. To this end, we assume that the individual features are linear functions of the process parameters, and use SpM to determine which set of process parameters to use.

In fields other than materials engineering, the 3+1 step model of functional expression in Figure 4 can be used to determine the properties to be found. Furthermore, a neural network model can be used to improve the performance of the Bayesian inference and SpM used in the 3+1 step model of functional expression. This is the universal paradigm of AI for science.

5. Summary

This review introduced the second neural network boom and its demise, which cannot be ignored when discussing the 2024 Nobel Prize in Physics, as well as the third neural network boom backed by steady academic progress. I also described the contributions of Japanese researchers whose work cannot be ignored, and presented a new perspective on information creation, statistical mechanics, and data-driven science. The 3+1 model of functional expression and three levels of data-driven science proposed by our group [52] was used to explain AI for materials engineering. This is an extension of the AI for science proposed by Hassabis, who was responsible for developing Alpha Go and was awarded the Nobel Prize in Chemistry in 2024.

The work that received this award is not only an outstanding achievement in physics as a basic science, but also a foundation for artificial intelligence research that goes beyond physics to social phenomena. It will have a great impact on human intellectual activities in the future.

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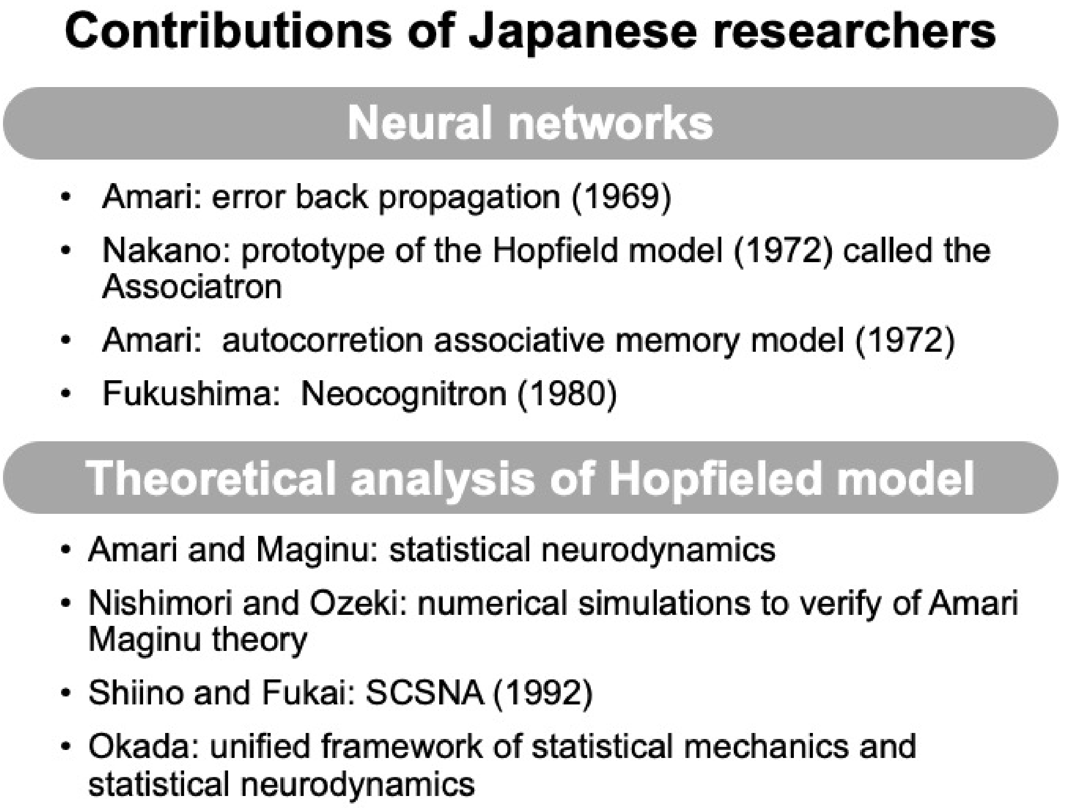


Contributions of Japanese researchers

Neural networks

- Amari: error back propagation (1969)
- Nakano: prototype of the Hopfield model (1972) called the Associatron
- Amari: autocorretion associative memory model (1972)
- Fukushima: Neocognitron (1980)

Theoretical analysis of Hopfieled model

- Amari and Maginu: statistical neurodynamics
- Nishimori and Ozeki: numerical simulations to verify of Amari Maginu theory
- Shiino and Fukai: SCSNA (1992)
- Okada: unified framework of statistical mechanics and statistical neurodynamics

Figure 1. Contributions of Japanese researchers.

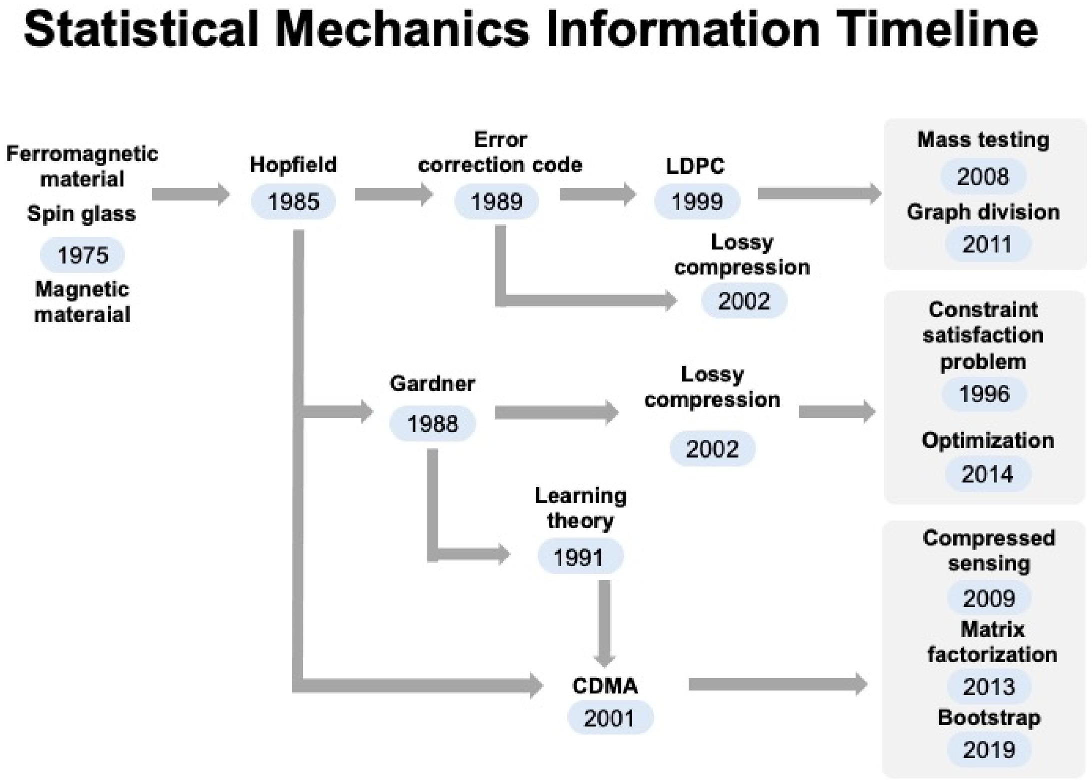


Figure 2. Statistical mechanical informatics timeline.

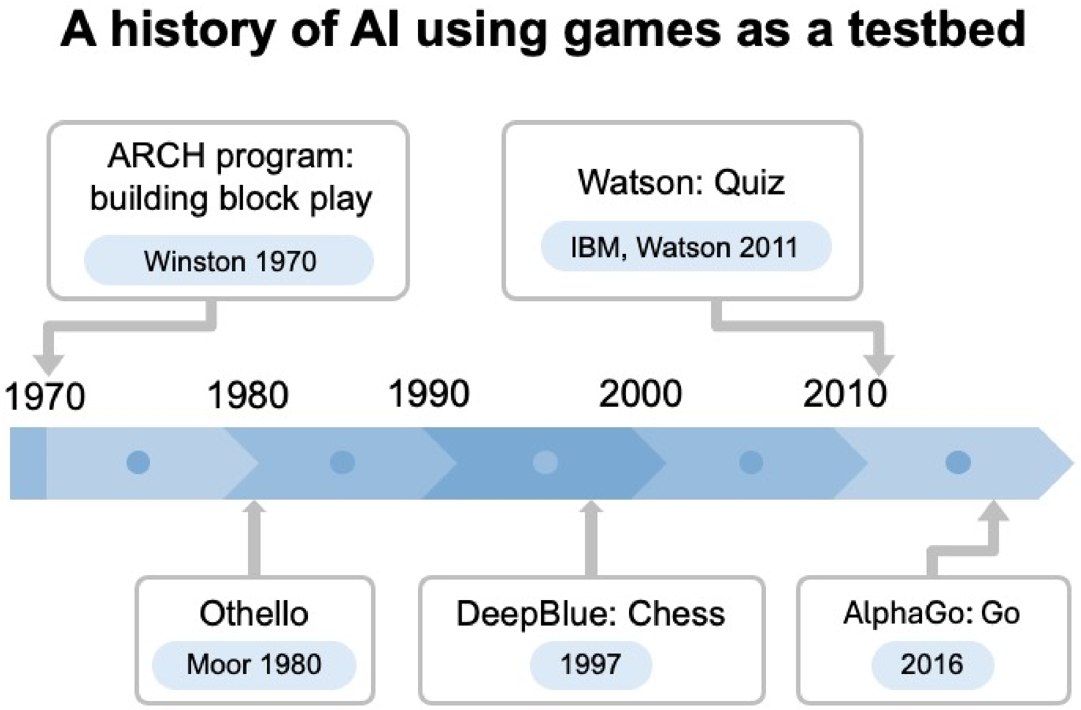


Figure 3. History of using games as AI test beds.

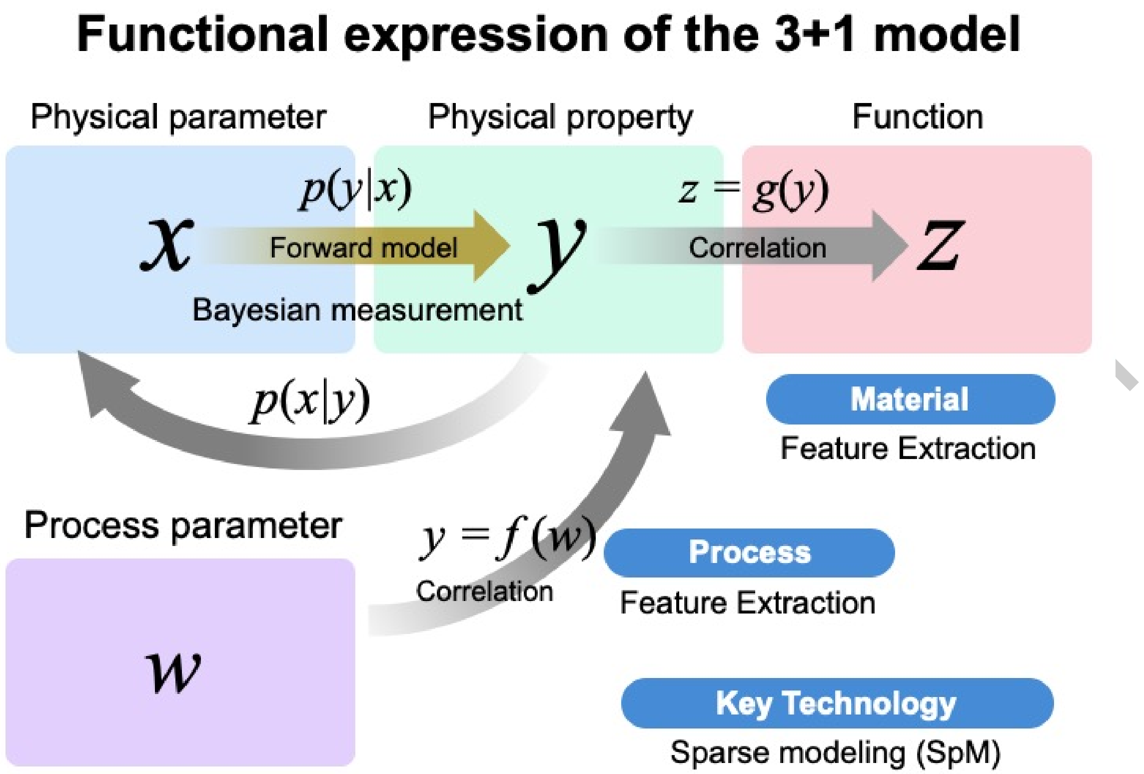


Figure 4. 3+1 model of functional expression.

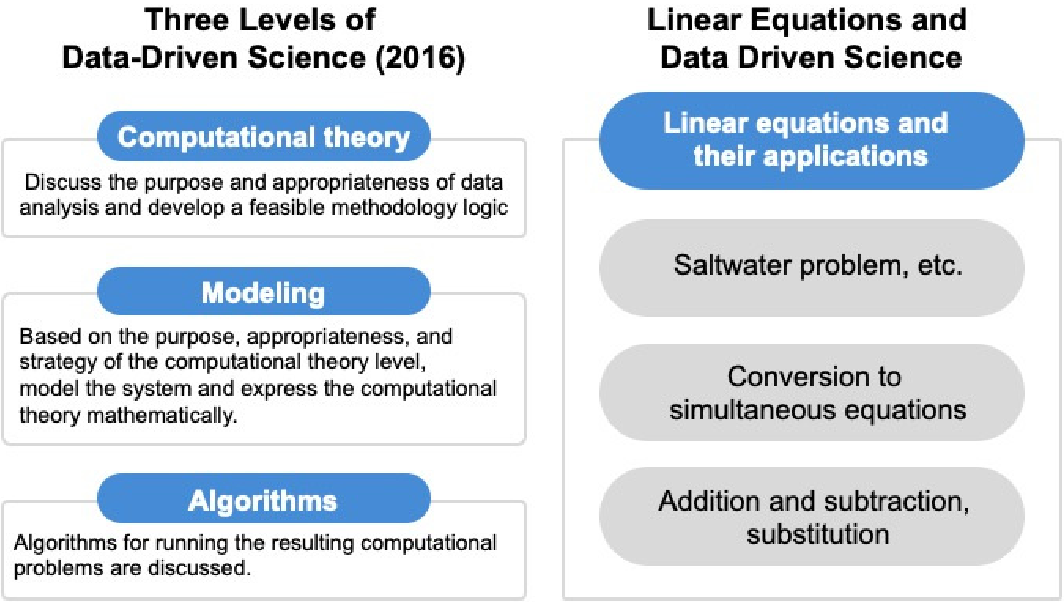
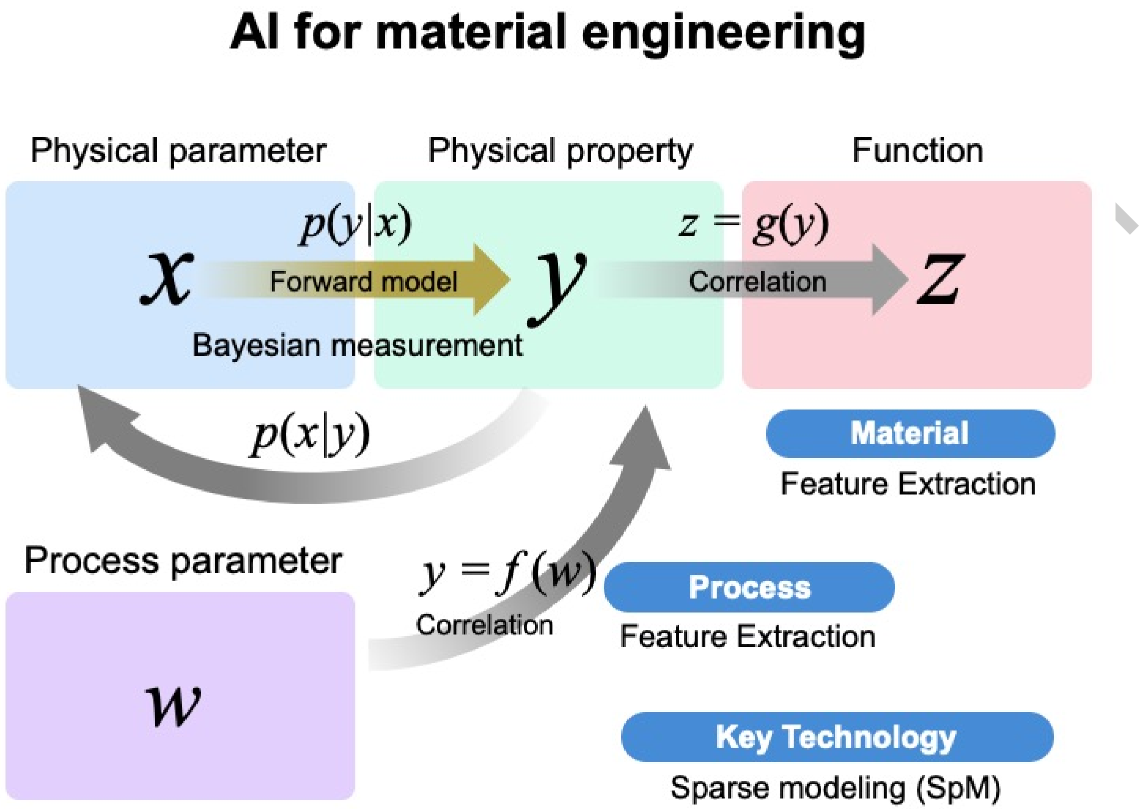


Figure 5. Three levels of data-driven science and linear equations.

Graphical Abstract



Biographical Note

Masato Okada has been a Professor at the Department of Complexity Science and Engineering, Graduate School of Frontier Sciences, The University of Tokyo, since 2004. His laboratory conducts demonstrative research in data-driven science in collaboration with numerous experimental groups, alongside theoretical studies on Bayesian measurement and sparse modeling. The primary application areas of data-driven science include condensed matter physics, materials science, and neuroscience.

Impact Statement:

This review discusses the 2024 Nobel Prizes in Physics and Chemistry with notable Japanese contributions, and recent advances in AI for science and material engineering, including the functional expression of the 3+1 model.