RESERCH PAPER

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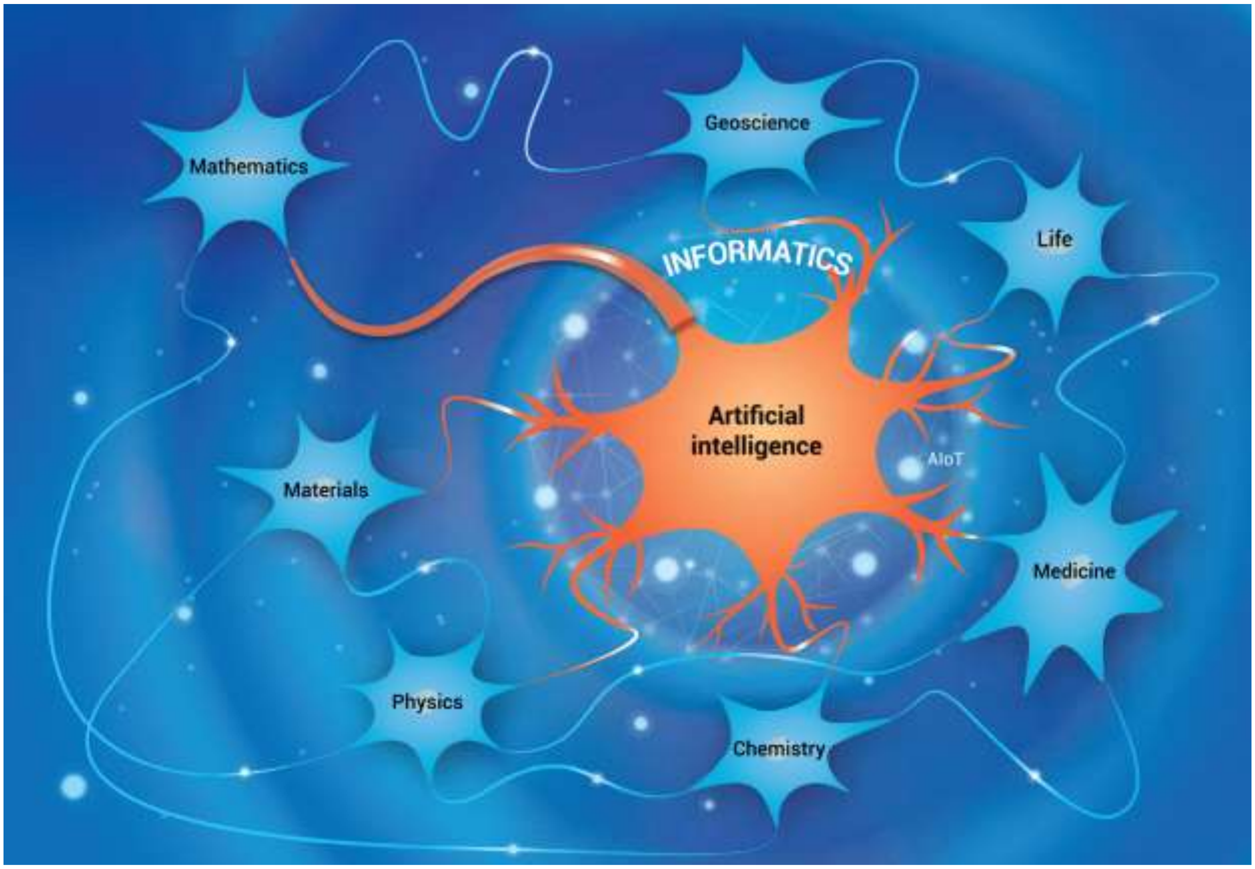
Artificial intelligence: A powerful paradigm for scientific research

- Introduction

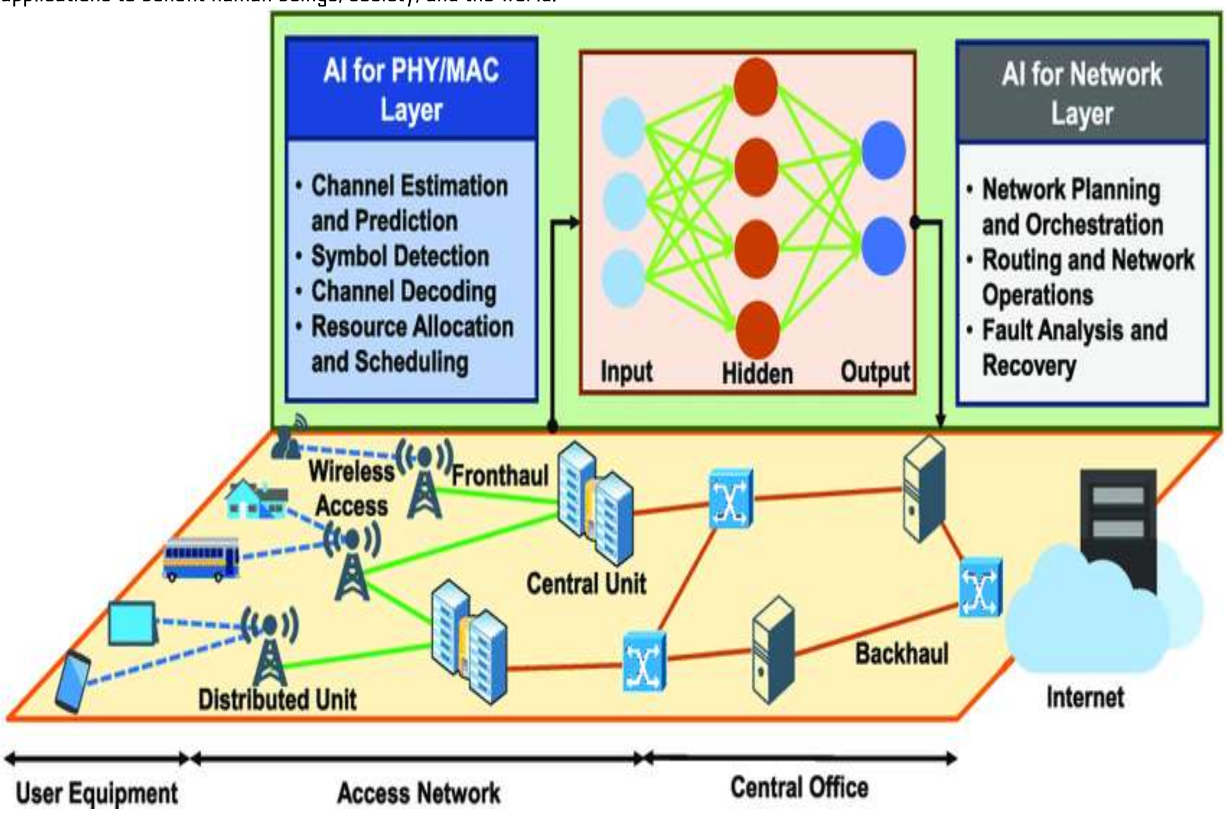
Artificial intelligence (AI) coupled with promising machine learning (ML) techniques well known from computer science is broadly affecting many aspects of various fields including science and technology, industry, and even our day-to-day life. The ML techniques have been developed to analyze high-throughput data with a view to obtaining useful insights categorizing, predicting, and making evidence-based decisions in novel ways, which will promote the growth of novel applications and fuel the sustainable booming of AI. This paper undertakes a comprehensive survey on the development and application of AI in different aspects of fundamental sciences, including information science, mathematics, medical science, materials science, geoscience, life science, physics, and chemistry. The challenges that each discipline of science meets, and the potentials of AI techniques to handle these challenges, are discussed in detail. Moreover, we shed light on new research trends entailing the integration of AI into each scientific discipline. The aim of this paper is to provide a broad research guideline on fundamental sciences with potential infusion of AI, to help motivate researchers to deeply understand the state-of-the-art applications of AI-based fundamental sciences, and thereby to help promote the continuous development of these fundamental sciences. However, it is difficult to define thinking clearly, because thinking is a subjective behavior. Turing then introduced an indirect method to verify whether a machine can think, the Turing test, which examines a machine's ability to show intelligence indistinguishable from that of human beings. A machine that succeeds in the test is qualified to be labeled as artificial intelligence (AI). AI refers to the simulation of human intelligence by a system or a machine. The goal of AI is to develop a machine that can think like humans and mimic human behaviors, including perceiving, reasoning, learning, planning, predicting, and so on. Intelligence is one of the main characteristics that distinguishes human beings from animals. With the interminable occurrence of industrial revolutions, an increasing number of types of machine types continuously replace human labor from all walks of life, and the imminent replacement of human resources by machine intelligence is the next big challenge to be overcome. Numerous scientists are focusing on the field of AI, and this makes the research in the field of AI rich and diverse. AI research fields include search algorithms, knowledge graphs, natural languages processing, expert systems, evolution algorithms, machine learning (ML), deep learning (DL), and so on. The general framework of AI is illustrated in Figure 1. The development process of AI includes perceptual intelligence, cognitive intelligence, and decision-making intelligence. Perceptual intelligence means that a machine has the basic abilities of vision, hearing, touch, etc., which are familiar to humans. Cognitive intelligence is a higher-level ability of induction, reasoning and acquisition of knowledge. It is inspired by cognitive science, brain science, and brain-like intelligence to endow machines with thinking logic and cognitive ability similar to human beings. Once a machine has the abilities of perception and cognition, it is often expected to make optimal decisions as human beings, to improve the lives of people, industrial manufacturing, etc. Decision intelligence requires the use of applied data science, social science, decision theory, and managerial science to expand data science, so as to make optimal decisions. To achieve the goal of perceptual intelligence, cognitive intelligence, and decision-making intelligence, the infrastructure layer of AI, supported by data, storage and computing power, ML algorithms, and AI frameworks is required. Then by training models, it is able to learn the internal laws of data for supporting and realizing AI applications. The application layer of AI is becoming more and more extensive, and deeply integrated with fundamental sciences, industrial manufacturing, human life, social governance, and cyberspace, which has a profound impact on our work and lifestyle.



- Background History

The beginning of modern AI research can be traced back to John McCarthy, who coined the term "artificial intelligence (AI)," during at a conference at Dartmouth College in 1956. This symbolized the birth of the A scientific field. Progress in the following years was astonishing. Many scientists and researchers focused on automated reasoning and applied AI for proving of mathematical theorems and solving of algebraic problems. One of the famous examples is Logic Theorist, a computer program written by Allen Newell, Herbert A. Simon, and Cliff Shaw, which proves 38 of the first 52 theorems in "Principia Mathematica" and provides more elegant proofs for some.2 These successes made many AI pioneers wildly optimistic, and underpinned the belief that fully intelligent machines would be built in the near future. However, they soon realized that there was still a long way to go before the end goals of human-equivalent intelligence in machine could come true. the logic-based programs. Another challenge was the lack of computational resources to compute more and more complicated problems. As a result, organizations and funders stopped supporting these under-delivering AI projects. AI came back to popularity in the 1980s, as several research institutions and universities invented a type of AI systems that summarizes a series of basic rules from expert knowledge to help non-experts make specific decisions. These systems are "expert systems." Examples are the XCON designed by Carnegie Mellon University and the MYCIN designed by Stanford University. The expert system derived logic rules from expert knowledge to solve problems in the real world for the first time. The core of AI research during this period is the knowledge that mademachines "smarter." However, the expert system gradually revealed several disadvantages, such as privacy technologies, lack of flexibility, poor versatility, expensive maintenance cost, and so on. At the same time, the Fifth Generation Computer Project, heavily funded by the Japanese government, failed tomeetmost of its original goals.Once again, the funding for AI research ceased, and AI was at the second lowest point of its life.

In 2006, Geoffrey Hinton and coworkers3,4 made a breakthrough in AI by proposing an approach of building deeper neural networks, as well as a way to avoid gradient vanishing during training. This reignited AI research, and DL algorithms have become one of themost active fields of AI research. DL is a subset of ML based on multiple layers of neural networks with representation learning,5 while ML is a part of AI that a computer or a program can use to learn and acquire intelligence without human intervention. Thus, "learn" is the keyword of this era of AI research. Big data technologies, and the improvement of computing power havemade deriving features and information frommassive data samplesmore efficient. An increasing number of new neural network structures and training methods have been proposed to improve the representative learning ability of DL, and to further expand it into general applications. Current DL algorithms match and exceed human capabilities on specific datasets in the areas of computer vision (CV) and natural language processing (NLP). AI technologies have achieved remarkable successes in all walks of life, and continued to show their value as backbones in scientific research and real-world applications. Within AI,ML is having a substantial broad effect across many aspects of technology and science: from computer science to geoscience to materials science, from life science to medical science to chemistry to mathematics and to physics, from management science to economics to psychology, and other data-intensive empirical sciences, asMLmethods have been developed to analyze high-throughput data to obtain useful insights, categorize, predict, andmake evidence-based decisions in novel ways. To train a system by presenting it with examples of desired input-output behavior, could be easier than to program it manually by predicting the desired response for all potential inputs. The following sections survey eight fundamental sciences, including information science (informatics), mathematics, medical science, materials science, geoscience, life science, physics, and chemistry, which develop or exploit AI techniques to promote the development of sciences and accelerate their applications to benefit human beings, society, and the world.



EXITING EVIDENCE -

AI aims to provide the abilities of perception, cognition, and decision-making for machines. At present, new research and applications in information science are emerging at an unprecedented rate, which is inseparable from the support by the AI infrastructure. As shown in Figure 2, the AI infrastructure layer includes data, storage and computing power,ML algorithms, and the AI framework. The perception layer enables machines have the basic ability of vision, hearing, etc. For instance, CV enables machines to "see" and identify objects, while speech recognition and synthesis helps machines to "hear" and recognize speech elements. The cognitive layer provides higher ability levels of induction, reasoning, and acquiring knowledge with the help of NLP,6 knowledge graphs,7 and continual learning.8 In the decision-making layer, AI is capable ofmaking optimal decisions, such as automatic planning,expert systems, and decision-supporting systems. Numerous applications of AI have had a profound impact on fundamental sciences, industrial manufacturing, human life, social governance, and cyberspace. The following subsections provide an overview of the AI framework, automatic machine learning (Auto ML) technology, and several state-of-the-art AI/ML applications in the information field.

The AI framework provides basic tools for AI algorithm Implementation

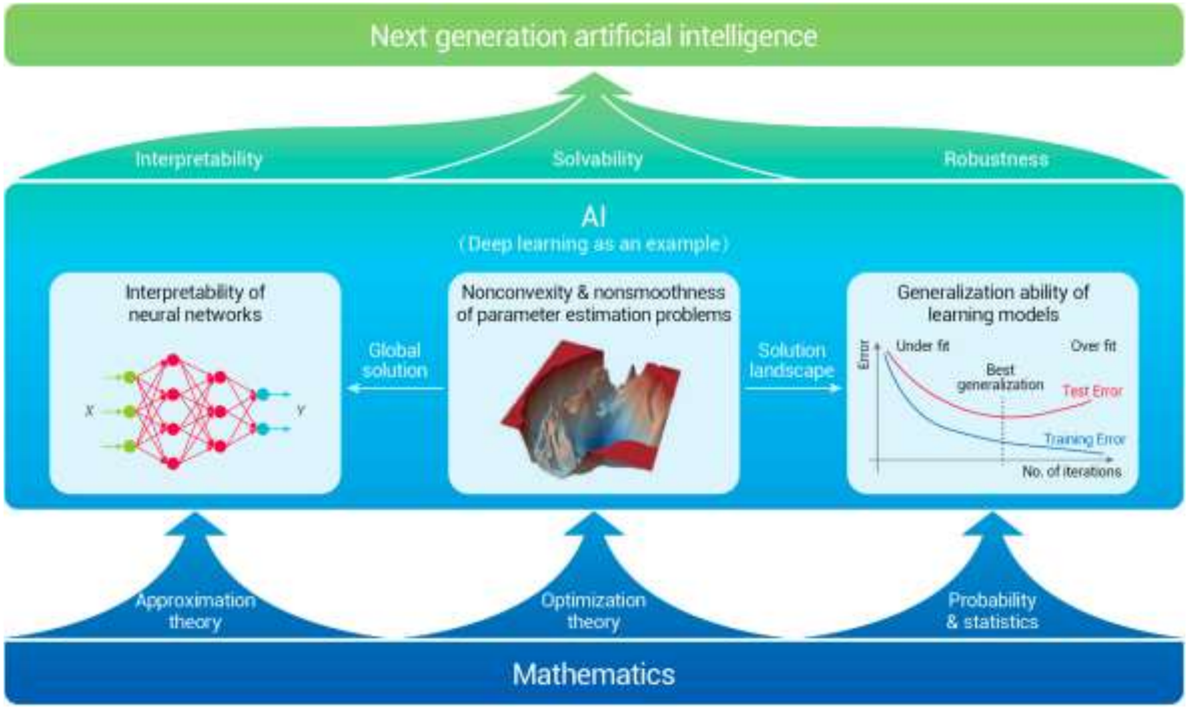
In the past 10 years, applications based on AI algorithms have played a significant role in various fields and subjects, on the basis of which the prosperity of the DL framework and platform has been founded. AI frameworks and platforms reduce the requirement of accessing AI technology by integrating the overall process of algorithm development, which enables researchers from different areas to use it across other fields, allowing them to focus on designing the structure of neural networks, thus providing better solutions to problems in their fields. At the beginning of the 21st century, only a few tools, such as MATLAB, OpenNN, and Torch, were capable of describing and developing neural networks. However, these tools were not originally designed for AImodels, and thus faced problems, such as complicated user API and lacking GPU support. During this period, using these frameworks demanded professional computer science knowledge and tedious work on model construction. As a solution, early frameworks of DL, such as Caffe,Chainer, and Theano, emerged, allowing users to conveniently construct complex deep neural networks (DNNs), such as convolutional neural networks (CNNs), recurrent neural networks (RNNs), and LSTM conveniently, and this significantly reduced the cost of applying AI models. Tech giants then joined the march in researching AI frameworks.9 Google developed the famous open-source framework, TensorFlow, while Facebook's AI research team released another popular platform, PyTorch, which is based on Torch; Microsoft Research published CNTK, and Amazon announced MXNet. Among them, TensorFlow, also the most representative framework,referred to Theano's declarative programming style, offering a larger space for graph-based optimization, while PyTorch inherited the imperative programming style of Torch, which is intuitive, user friendly, more flexible, and easier to be traced. Asmodern AI frameworks and platforms are beingwidely applied, practitioners can now assemble models swiftly and conveniently by adopting various building block sets and languages specifically suitable for given fields. Polished over time, these platforms gradually developed a clearly defined user API, the ability formulti-GPU training and distributed training, as well as a variety of model zoos and tool kits for specific tasks.10 Looking forward, there are a few trends that may become the mainstream of next-generation framework development. (1) Capability of super-scalemodel training. With the emergence of models derived fromTransformer, such as BERT and GPT-3, the ability of training largemodels has become an ideal feature of the DL framework. It requires AI frameworks to train effectively under the scale of hundreds or even thousands of devices. (2) Unified API standard. The APIs of many frameworks are generally similar but slightly different at certain points. This leads to some difficulties and unnecessary learning efforts, when the user attempts to shift from one framework to another. The API of some frameworks, such as JAX, has already become compatible with Numpy standard, which is familiar tomost practitioners. Therefore, a unified API standard for AI frameworks may gradually come into being in the future. (3) Universal operator optimization. At present, kernels of DL operator are implemented either manually or based on third-party libraries. Most third-party libraries are developed to suit certain hardware platforms, causing large unnecessary spending when models are trained or deployed on different hardware platforms. The development speed of new DL algorithms is usually much faster than the update rate of libraries, which often makes new algorithms to be beyond the range of libraries' suppor.

AI for AI—AutoML

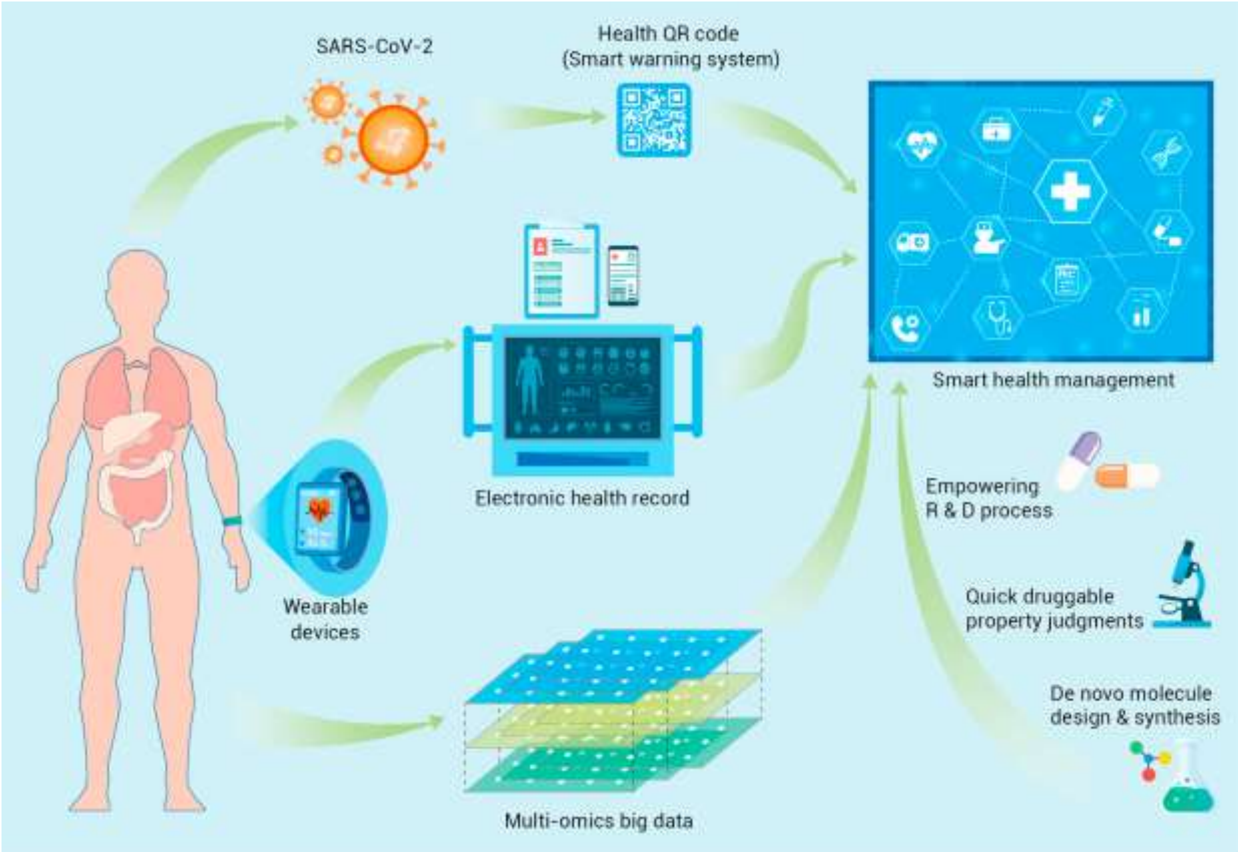
AutoML aims to study how to use evolutionary computing, reinforcement learning (RL), and other AI algorithms, to automatically generate specified AI algorithms. Research on the automatic generation of neural networks has existed before the emergence of DL, e.g., neural evolution.13 The main purpose of neural evolution is to allow neural networks to evolve according to the principle of survival of the fittest in the biological world. Through selection, crossover, mutation, and other evolutionary operators, the individual quality in a population is continuously improved and, finally, the individual with the greatest fitness represents the best neural network. The biological inspiration in this field lies in the evolutionary process of human brain neurons. The human brain has such developed learning and memory functions that it cannot do without the complex neural network system in the brain. The whole neural network system of the human brain benefits from a long evolutionary process rather than gradient descent and back propagation. In the era of DL, the application of AI algorithms to automatically generate DNN has attracted more attention and, gradually, developed into an important direction of AutoML research: neural architecture search. The implementation methods of neural architecture search are usually divided into the RL-based method and the evolutionary algorithm-based method. In the RL-based method, an RNN is used as a controller to generate a neural network structure layer by layer, and then the network is trained, and the accuracy of the verification set is used as the reward signal of the RNN to calculate the strategy gradient. During the iteration, the controller will give the neural network, with higher accuracy, a higher probability value, so as to ensure that the strategy function can output the optimal network structure.

AI enabling more powerful and intelligent nanophotonics

Nanophotonic components have recently revolutionized the field of optics via metamaterials/metasurfaces by enabling the arbitrary manipulation of light-matter interactions with subwavelength meta-atoms or meta-molecules. 20–22 The conventional design of such components involves generally forward modeling, i.e., solving Maxwell's equations based on empirical and intuitive nanostructures to find corresponding optical properties, as well as the inverse design of nanophotonic devices given an on-demand optical response. The trans-dimensional feature of macro-optical components consisting of complex nano-antennas makes the design process very time consuming, computationally expensive, and even numerically prohibitive, such as device size and complexity increase. DL is an efficient and automatic platform, enabling novel efficient approaches to designing nanophotonic devices with high-performance and versatile functions. Here, we present briefly the recent progress of DL-based nanophotonics and its wide-ranging applications. DL was exploited for forward modeling at first using a DNN.23 The transmission or reflection coefficients can be well predicted after training on huge datasets. To improve the prediction accuracy of DNN in case of small datasets, transfer learning was introduced to migrate knowledge between different physical scenarios, which greatly reduced the relative error.
Furthermore, a CNN and an RNN were developed for the prediction of optical properties from arbitrary structures using images.24 The CNN-RNN combination successfully predicted the absorption spectra fromthe given input structural images. In inverse design of nanophotonic devices, there are three different paradigms of DL methods, i.e., supervised, unsupervised, and RL.25 Supervised learning has been utilized to design structural parameters for the pre-defined geometries, such as tandem DNN and bidirectional DNNs. Unsupervised learning methods learn by themselves without a specific target, and thus are more accessible to discovering new and arbitrary patterns26 in completely new data than supervised learning. A generative adversarial network (GAN)-based approach, combining conditional GANs and Wasserstein GANs, was proposed to design freeform all-dielectricmultifunctionalmetasurfaces. RL, especially double-deep Q-learning, powers up the inverse design of high-performance nanophotonic devices.27 DL has endowed nanophotonic devices with better performance and more emerging applications



The optimization problems of parameter estimation In general, the optimization problem of estimating parameters of certain DNNs is in practice highly nonconvex and often nonsmooth. Can the global minimizers be expected? What is the landscape of local minimizers? How does one handle the nonsmoothness? All these questions are nontrivial from an optimization perspective. Indeed, numerous works and experiments demonstrate that the optimization for parameter estimation in DL is itself a much nicer problem than once thought; see, e.g., Goodfellow et al. 44 As a consequence, the study on the solution landscape (Figure 3), also known as loss surface of neural networks, is no longer supposed to be inaccessible and can even in turn provide guidance for global optimization. Interested readers can refer to the survey paper (Sun et al.45) for recent progress in this aspect. Recent studies indicate that nonsmooth activation functions, e.g., rectified linear units, are better than smooth ones in finding sparse solutions.However, the chain rule does not work in the case that the activation functions are nonsmooth, which then makes the widely used stochastic gradient (SG)-based approaches not feasible in theory. Taking approximated gradients at nonsmooth iterates as a remedy ensures that SG-typemethods are still in extensive use, but that the numerical evidence has also exposed their limitations. Also, the penalty-based approaches proposed by Cui et al.46 and Liu et al.47 provide a new direction to solve the nonsmooth optimization problems efficiently.



AI doctor based on electronic medical records

For medical history data, it is inevitable to mention Doctor Watson, developed by the Watson platformof IBM, andModernizingMedicine, which aims to solve oncology, and is now adopted by CVS & Walgreens in the US and various medical organizations in China as well. Doctor Watson takes advantage of the NLP performance of the IBM Watson platform, which already collected vast data of medical history, as well as prior knowledge in the literature for reference. After inputting the patients' case, Doctor Watson searches themedical history reserve and forms an elementary treatment proposal, which will be further ranked by prior knowledge reserves.With the multiple models stored, Doctor Watson gives the final proposal as well as the confidence of the proposal. However, there are still problems for such AI doctors because,51 as they rely on prior experience from US hospitals, the proposal may not be suitable for other regions with different medical insurance policies. Besides, the knowledge updating of the Watson platformalso relies highly on the updating of the knowledge reserve, which still needs manual work.

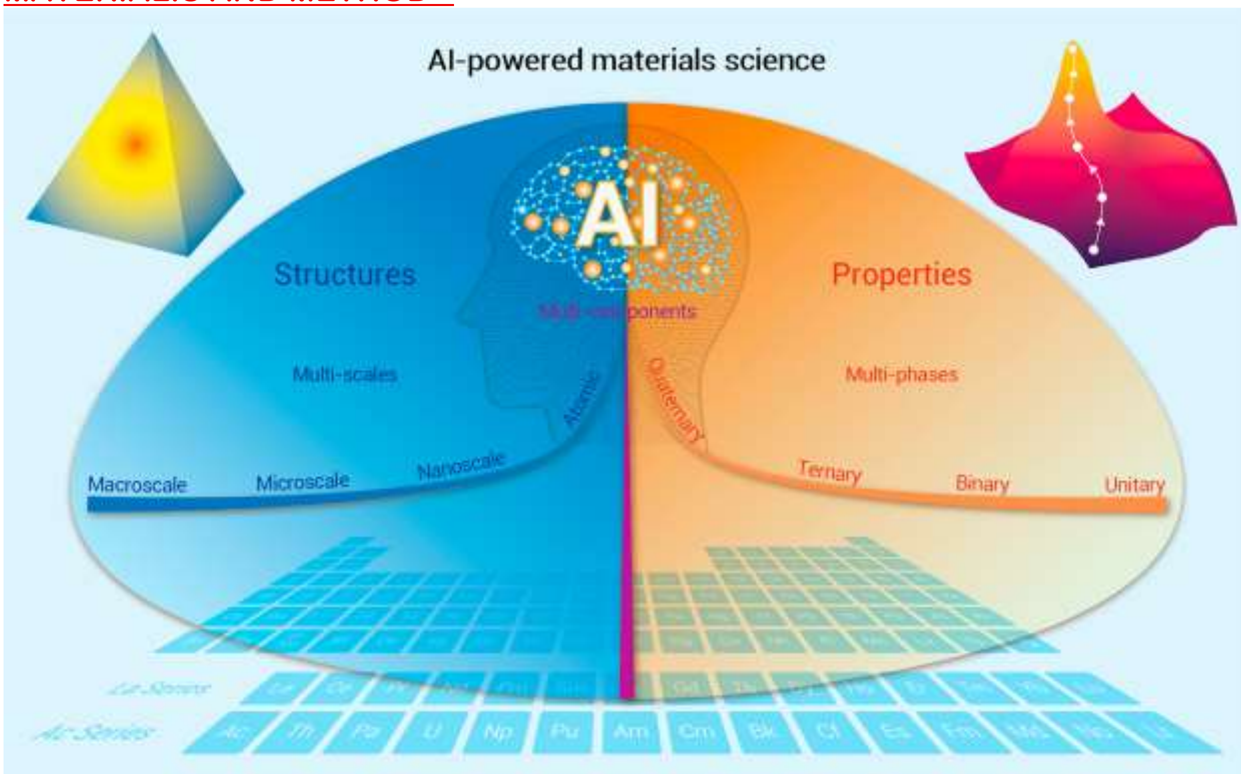
Biomarker discovery with AI

High-dimensional data, including multi-omics data, patient characteristics, medical laboratory test data, etc., are often used for generating various predictive or prognosticmodels through DL or statisticalmodelingmethods. For instance, the COVID-19 severity evaluationmodel was built throughML using proteomic andmetabolomic profiling data of sera55; using integrated genetic, clinical, and demographic data, Taliaz et al. built an ML model to predict patient response to antidepressant medications56; prognostic models for multiple cancer types (such as liver cancer, lung cancer, breast cancer, gastric cancer, colorectal cancer, pancreatic cancer, prostate cancer, ovarian cancer, lymphoma, leukemia, sarcoma, melanoma, bladder cancer, renal cancer, thyroid cancer, head and neck cancer, etc.) were constructed through DL or statistical methods, such as least absolute shrinkage and selection operator （LASSO） , combined with Cox proportional hazards regression model using genomic data

Image-based medical AI

Medical image AI is one of the most developedmature areas as there are numerous models for classification, detection, and segmentation tasks in CV.

MATERIALIS AND METHOD –



demonstrated for efficient and accurate prediction of functional molecular materials, with desired semiconducting properties or redox stability for applications in organic thin-film transistors, organic solar cells, or lithium-ion batteries. 73 It is meaningful to adopt automation tools for quick experimental testing of potential materials and utilize high-performance computing to calculate their bulk, interface, and defect-related properties.74 The effective convergence of automation, computing, andML can greatly speed up the discovery of materials. In the future, with the aid of AI techniques, it will be possible to accomplish the design of superconductors, metallic glasses, solder alloys, high-entropy alloys, high-temperature superalloys, thermoelectric materials, two-dimensional materials, magnetocaloric materials, polymeric bio-inspired materials, sensitive composite materials, and topological (electronic and phonon) materials, and so on. In the past decade, topological materials have ignited the research enthusiasm of condensed matter physicists, materials scientists, and chemists, as they exhibit exotic physical properties with potential applications in electronics, thermoelectrics, optics, catalysis, and energy-related fields. From the most recent predictions, more than a quarter of all inorganic materials in nature are topologically nontrivial. The establishment of topological electronic materials databases75–77 and topological phononic materials databases78 using high-throughput methods will help to accelerate the screening and experimental discovery of new topological materials for functional applications. It is recognized that large-scale high-quality datasets are required to practice AI. Great efforts have also been expended in building high-quality materials science databases. As one of the top-ranking databases of its kind, the "atomly.net" materials data infrastructure,79 has calculated the properties of more than 180,000 inorganic compounds, including their equilibrium structures, electron energy bands, dielectric properties, simulated diffraction patterns, elasticity tensors, etc. As such, the atomly.net database has set a solid foundation for extending AI into the area of materials science research. The X-ray diffraction (XRD)- matcher model of atomly.net uses ML to match and classify the experimental XRD to the simulated patterns. Very recently, by using the dataset from atomly.net, an accurate AI model was built to rapidly predict the formation energy of almost any given compound to yield a fairly good predictive ability.

AI for materials and materials for AI

The coming decade will continue to witness the development of advanced ML algorithms, newly emerging data-driven AI methodologies, and integrated technologies for facilitating structure design and property prediction, as well as to accelerate the discovery, design, development, and deployment of advanced materials into existing and emerging industrial sectors. At this moment, we are facing challenges in achieving accelerated materials research through the integration of experiment, computation, and theory. The great MGI, proposed for high-level materials research, helps to promote this process, especially when it is assisted by AI techniques. Still, there is a long way to go for the usage of these advanced functional materials in future-generation electric chips and devices to be realized. More materials and functional effects need to be discovered or improved by the developing AI techniques. Meanwhile, it is worth noting that materials are the core components of devices and chips that are used for construction of computers or machines for advanced AI systems. The rapid development of newmaterials, especially the emergence of flexible, sensitive, andsmartmaterials, is of great importance for a broad range of attractive technologies, such as flexible circuits, stretchable tactile sensors, multifunctional actuators, transistor-based artificial synapses, integrated networks of semiconductor/quantum devices, intelligent robotics, human-machine interactions, simulated muscles, biomimetic prostheses, etc. These promising materials, devices, and integrated technologies will greatly promote the advancement of AI systems toward wide applications in human life. Once the physical circuits are upgraded by advanced functional or smart materials, AI techniques will largely promote the developments and applications of all disciplines.

Multiple challenges in the development of geoscience

There are some traits of geoscience development that restrict the applicability of fundamental algorithms for knowledge discovery: (1) inherent challenges of geoscience processes, (2) limitation of geoscience data collection, and (3) uncertainty in samples and ground truth.88–90 Amorphous boundaries generally exist in geoscience objects between space and time that are not as well defined as objects in other fields. Geoscience phenomena are also significantly multivariate, obey nonlinear relationships, and exhibit spatiotemporal structure and non-stationary characteristics. Except for the inherent challenges of geoscience observations, themassive data at multiple dimensions of time and space, with different levels of incompleteness, noise, and uncertainties, disturb processes in geoscience. For supervised learning approaches, there are other difficulties owing to the lack of gold standard ground truth and the "small size" of samples (e.g., a small amount of historical data with sufficient observations) in geoscience applications.

Usage of AI technologies as efficient approaches to promote the

geoscience processes Geoscientists continually make every effort to develop better techniques for simulating the present status of the Earth system (e.g., how much greenhouse gases are released into the atmosphere), and the connections between andwithin its subsystems (e.g., how does the elevated temperature influence the ocean ecosystem). Viewed from the perspective of geoscience, newly emerging approaches, with the aid of AI, are a perfect combination for these issues in the application of geoscience: (1) characterizing objects and events91; (2) estimating geoscience variables from observations92; (3) forecasting geoscience variables according to long-term observations85; (4) exploring geoscience data relationships93; and (5) causal discovery and causal attribution.94 While characterizing geoscience objects and events using traditional methods are primarily rooted in hand-coded features, algorithms can automatically detect the data by improving the performance with pattern-mining techniques. However, due to spatiotemporal targets with vague boundaries and the related uncertainties, it can be necessary to advance pattern-mining methods that can explain the temporal and spatial characteristics of geoscience data when characterizing different events and objects. To address the non-stationary issue of geoscience data, AI-aided algorithms have been expanded to integrate the holistic results of professional predictors and engender robust estimations of climate variables (e.g., humidity and temperature). Furthermore, forecasting long-term trends of the current situation in the Earth system using AI-enabled technologies can simulate future scenarios and formulate early resource planning and adaptation policies. Mining geoscience data relationships can help us seize vital signs of the Earth system and promote our understanding of geoscience developments. Of great interest is the advancement of AI-decisionmethodology with uncertain prediction probabilities, engendering vague risks with poorly resolved tails, signifying the most extreme, transient, and rare events formulated by model sets, which supports various cases to improve accuracy and effectiveness.

AI technologies for optimizing the resource management in geoscience

Currently, AI can perform better than humans in some well-defined tasks. For example, AI techniques have been used in urbanwater resource planning, mainly due to their remarkable capacity for modeling, flexibility, reasoning, and forecasting the water demand and capacity. Design and application of an Adaptive Intelligent Dynamic Water Resource Planning system, the subset of AI for sustainable water resource management in urban regions, largely prompted the optimization of water resource allocation, will finally minimize the operation costs and improve the sustainability of environmental management95 (Figure 6). Also, meteorology requires collecting tremendous amounts of data on many different variables, such as humidity, altitude, and temperature; however, dealing with such a huge dataset is a big challenge. 96 An AI-based technique is being utilized to analyze shallow-water reef images, recognize the coral color—to track the effects of climate change, and to collect humidity, temperature, and CO2 data—to grasp the health of our ecological environment.97 Beyond AI's capabilities for meteorology, it can also play a critical role in decreasing greenhouse gas emissions originating from the electric-power sector. Comprised of production, transportation, allocation, and consumption of electricity, many opportunities exist in the electric- power sector for AI applications, including speeding up the development of new clean energy, enhancing system optimization and management, improving electricity-demand forecasts and distribution, and advancing systemmonitoring. 98 Newmaterials may even be found, with the auxiliary of AI, for batteries to store energy or materials and absorb CO2 from the atmosphere. 99 Although traditional fossil fuel operations have been widely used for thousands of years, AI techniques are being used to help explore the development of more potential sustainable energy sources for the development (e.g., fusion technology)

AI as a building block to promote development in geoscience

The Earth's system is of significant scientific interest, and affects all aspects of life.106 The challenges, problems, and promising directions provided by AI are definitely not exhaustive, but rather, serve to illustrate that there is great potential for future AI research in this important field. Prosperity, development, and popularization of AI approaches in the geosciences is commonly driven by a posed scientificquestion,and thebestway tosucceed is that AI researchers work closely with geoscientists at all stages of research. That is because the geoscientists can better understand which scientific question is important and novel, which sample collection process can reasonably exhibit the inherent strengths, which datasets and parameters can be used to answer that question, and which pre-processing operations are conducted, such as removing seasonal cycles or smoothing. Similarly, AI researchers are better suited to decide which data analysis approaches are appropriate and available for the data, the advantages and disadvantages of these approaches, and what the approaches actually acquire. Interpretability is also an important goal in geoscience because, if we can understand the basic reasoning behind the models, patterns, or relationships extracted from the data, they can be used as building blocks in scientific knowledge discovery. Hence, frequent communication between the researchers avoids long detours and ensures that analysis results are indeed beneficial to both geoscientists and AI researchers.

Mutual inspiration between AI and neuroscience

In the past decades, neuroscience concepts have been introduced into ML algorithms and played critical roles in triggering several important advances in AI. For example, the origins of DL methods lie directly in neuroscience,5 which further stimulated the emergence of the field of RL.108 The current state-of-the-art CNNs incorporate several hallmarks of neural computation, including nonlinear transduction, divisive normalization, and maximum-based pooling of inputs,109 which were directly inspired by the unique processing of visual input in the mammalian visual cortex.110 By introducing the brain's attentional mechanisms, a novel network has been shown to produce enhanced accuracy and computational efficiency at difficult multi-object recognition tasks than conventional CNNs.111 Other neuroscience findings, including the mechanisms underlying working memory, episodic memory, and neural plasticity, have inspired the development of AI algorithms that address several challenges in deep networks.108 These algorithms can be directly implemented in the design and refinement of the brain-machine interface and neuroprostheses.

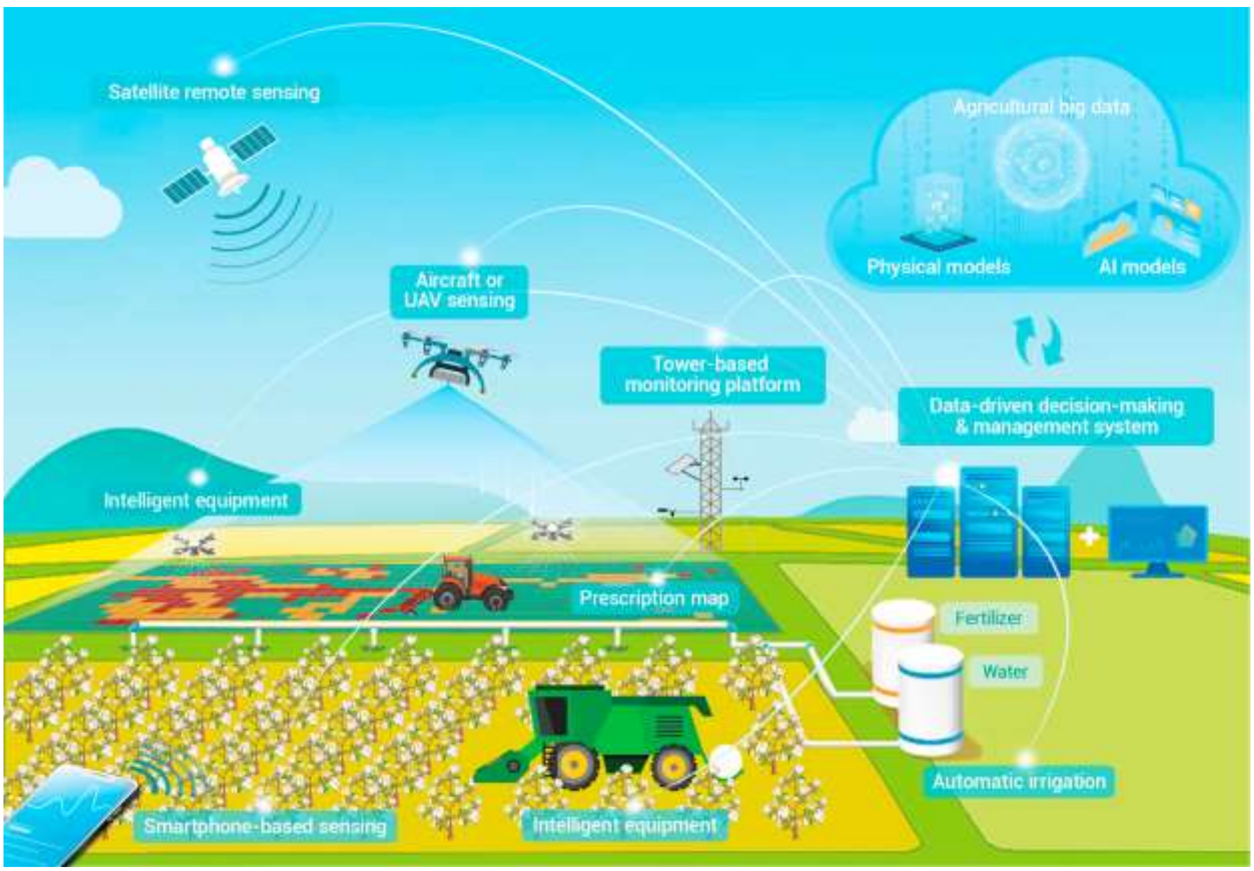
On the other hand, insights fromAI research have the potential to offer new perspectives on the basics of intelligence in the brains of humans and other species. Unlike traditional neuroscientists, AI researchers can formalize the concepts of neural mechanisms in a quantitative language to extract their necessity and sufficiency for intelligent behavior. An important illustration of such exchange is the development of the temporal-difference (TD) methods in RLmodels and the resemblance of TD-form learning in the brain.112 Therefore, the China Brain Project covers both basic research on cognition and translational research for brain disease and brain-inspired intelligence technology.

AI for omics big data analysis

Currently, AI can perform better than humans in some well-defined tasks, such as omics data analysis and smart agriculture. In the big data era, there are many types of data (variety), the volume of data is big, and the generation of data (velocity) is fast. The high variety, big volume, and fast velocity of data makes having it a matter of big value, but also makes it difficult to analyze the data. Unlike traditional statistics-based methods, AI can easily handle big data and reveal hidden associations. In genetics studies, there are many successful applications of AI.115 One of the key questions is to determine whether a single amino acid polymorphism is deleterious.116 There have been sequence conservation-based SIFT117 and network-based SySAP,118 but all thesemethods have met bottlenecks and cannot be further improved. Sundaram et al. developed PrimateAI, which can predict the clinical outcome of mutation based on DNN.

AI makes modern agriculture smart

Agriculture is entering a fourth revolution, termed agriculture 4.0 or smart agriculture, benefiting from the arrival of the big data era as well as the rapid progress of lots of advanced technologies, in particularML,modern information, and communication technologies.134,135 Applications of DL, information, and sensing technologies in agriculture cover thewhole stages of agricultural production, including breeding, cultivation, and harvesting. Traditional breeding usually exploits genetic variations by searching natural variation or artificialmutagenesis. However, it is hard for eithermethod to expose the whole mutation spectrum. Using DL models trained on the existing variants, predictions can be made on multiple unidentified gene loci.136 For example, an ML method, multi-criteria rice reproductive gene predictor, was developed and applied to predict coding and lincRNA genes associated with reproductive processes in rice.137 Moreover, models trained in species with well-studied genomic data (such as Arabidopsis and rice) can also be applied to other specieswith limited genome information (such aswild strawberry and soybean).138 In most cases, the links between genotypes and phenotypes are more complicated than we expected. One gene can usually respond to multiple phenotypes, and one trait is generally the product of the synergism between multi-genes and multi-development. For this reason, multi-traits DLmodels were developed and enabled genomic editing in plant breeding.



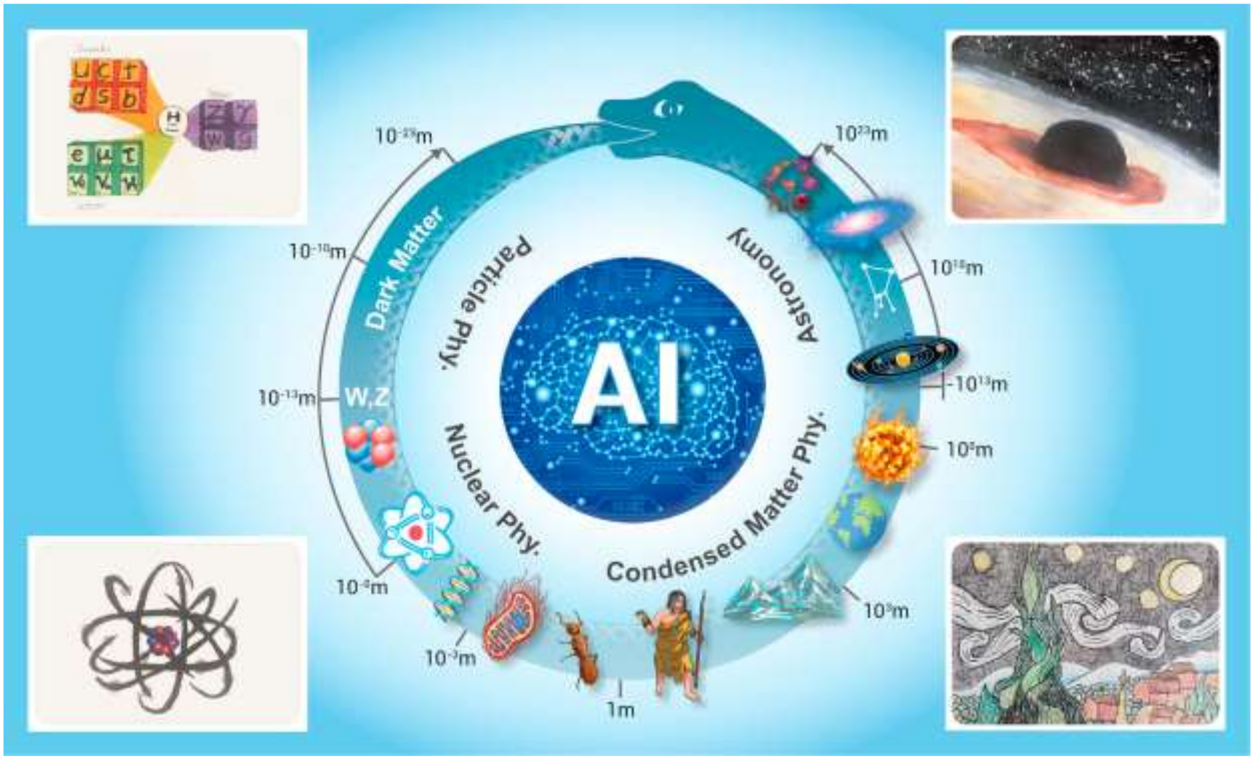
information, owing to its strong capability for feature representation and superiority in capturing the essential relation between observation data and agronomy parameters or crop traits.135,143 Integration of DL and big data for agriculture has demonstrated the most disruptive force, as big as the green revolution. As shown in Figure 7, for possible application a scenario of smart agriculture, multi-source satellite remote sensing data with various geo- and radio-metric information, as well as abundance of spectral information from UV, visible, and shortwave infrared to microwave regions, can be collected. In addition, advanced aircraft systems, such as unmanned aerial vehicles with multi/hyper-spectral cameras on board, and smartphonebased portable devices, will be used to obtain multi/hyper-spectral data in specific fields. All types of data can be integrated by DL-based fusion techniques for different purposes, and then shared for all users for cloud computing. On the cloud computing platform, different agriculture remote sensing models developed by a combination of data-driven ML methods and physical models, will be deployed and applied to acquire a range of biophysical and biochemical parameters of crops, which will be further analyzed by a decision-making and prediction system to obtain the current water/nutrient stress, growth status, and to predict future development. As a result, an automatic or interactive user service platform can be accessible to make the correct decisions for appropriate actions through an integrated irrigation and fertilization system. Furthermore, DL presents unique advantages in specific agricultural applications, such as for dense scenes, that increase the difficulty of artificial planting and harvesting. It is reported that CNNs and Autoencoder models, trained with image data, are being used increasingly for phenotyping and yield estimation,144 such as counting fruits in orchards, grain recognition and classification, disease diagnosis, etc.145–147 Consequently, this may greatly liberate the labor force. Speeding up simulations and identifications of particles with AI There aremany applications or explorations of applications of AI in particle physics. We cannot cover all of them here, but only use lattice quantum chromodynamics (LQCD) and the experiments on the Beijing spectrometer (BES) and the large hadron collider (LHC) to illustrate the power of ML in both theoretical and experimental particle physics. LQCD studies the nonperturbative properties of QCD by using Monte Carlo simulations on supercomputers to help us understand the strong interaction that binds quarks together to form nucleons. Markov chain Monte Carlo simulations commonly used in LQCD suffer from topological freezing and critical slowing down as the simulations approach the real situation of the actual world. New algorithms with the help of DL are being proposed and tested to overcome those difficulties.148,149 Physical observables are extracted from LQCD data, whose signal-to-noise ratio

AI IN PHYSICS

The scale of modern physics ranges from the size of a neutron to the size of the Universe (Figure 8). According to the scale, physics can be divided into four categories: particle physics on the scale of neutrons, nuclear physics on the scale of atoms, condensedmatter physics on the scale of molecules, and cosmic physics on the scale of the Universe. AI, also called ML, plays an important role in all physics in different scales, since the use of the AI algorithm will be the main trend in data analyses, such as the reconstruction and analysis of images.

AI-aided condensed matter physics

AI opens up a new avenue for physical science, especially when a trove of data is available. Recent works demonstrate that ML provides useful insights to improve the density functional theory (DFT), in which the singleelectron picture of the Kohn-Sham scheme has the difficulty of taking care of the exchange and correlation effects of many-body systems. Yu et al. proposed a Bayesian optimization algorithm to fit the Hubbard parameter, and the new method can find the optimal Hubbard U through a self-consistent process with good efficiency compared with the linear response method,157 and boost the accuracy to the near-hybrid-functional- level. Snyder et al. developed an ML density functional for a 1D non-interacting non-spin-polarized fermion system to obtain significantly improved kinetic energy. This method enabled a direct approximation of the kinetic energy of a quantum system and can be utilized in orbital-free DFT modeling, and can even bypass the solving of the Kohn-Sham equation— while maintaining the precision to the quantum chemical level when a strong correlation term is included. Recently, FermiNet showed that the many-body quantum mechanics equations can be solved via AI. AI models.



AI makes nuclear physics powerful

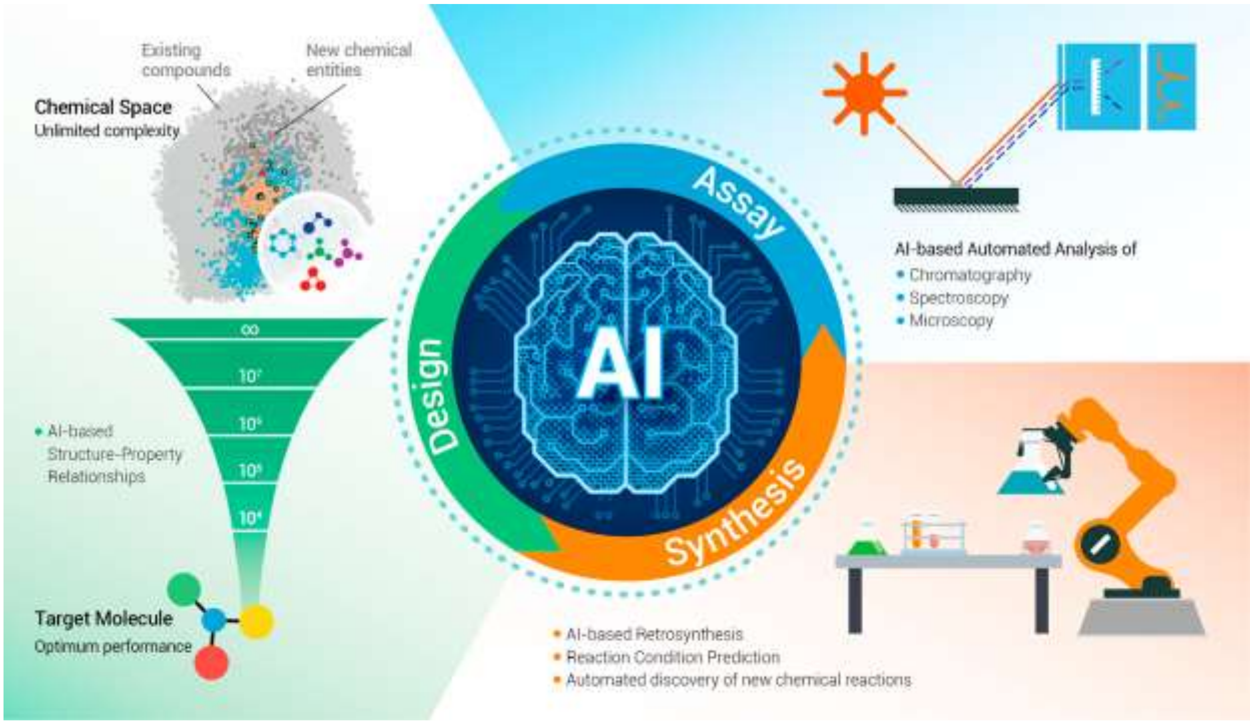
Cosmic raymuon tomography (Muography)155 is an imaging graphe technology using natural cosmic raymuon radiation rather than artificial radiation to reduce the dangers. As an advantage, this technology can detect high-Z materials without destruction, as muon is sensitive to high-Z materials. The Classification Model Algorithm (CMA) algorithm is based on the classification in the supervised learning and gray system theory, and generates a binary classifier designing and decision function with the input of the muon track, and the output indicates whether the material exists at the location. The AI helps the user to improve the efficiency of the scanning time with muons also show advantages of capturing the interatom force field. In 2010, the Gaussian approximation potential (GAP)158 was introduced as a powerful interatomic force field to describe the interactions between atoms. GAP uses kernel regression and invariant many-body representations, and performs quite well. For instance, it can simulate crystallization of amorphous crystals under high pressure fairly accurately. By employing the smooth overlap of the atomic position kernel (SOAP),159 the accuracy of the potential can be further enhanced and, therefore, the SOAP-GAP can be viewed as a field-leading method for AI molecular dynamic simulation. There are also several other well-developed AI interatomic potentials out there, e.g., crystal graph CNNs provide a widely applicable way of vectorizing crystalline materials; SchNet embeds the continuous-filter convolutional layers into its DNNs for easing molecular dynamic as the potentials are space continuous; DimeNet constructs the directional message passing neural network by adding not only the bond length between atoms but also the bond angle, the dihedral angle, and the interactions between unconnected atoms into the model to obtain good accuracy.

AI helps explore the Universe

AI is one of the newest technologies, while astronomy is one of the oldest sciences.When the twomeet, new opportunities for scientific breakthroughs are often triggered. Observations and data analysis play a central role in astronomy. The amount of data collected by modern telescopes has reached unprecedented levels, even the most basic task of constructing a catalog has become challenging with traditional source-finding tools.160 Astronomers have developed automated and intelligent source-finding tools based on DL, which not only offer significant advantages in operational speed but also facilitate a comprehensive understanding of the Universe by identifying particular forms of objects that cannot be detected by traditional software and visual inspection.160,161 More than a decade ago, a citizen science project called "Galaxy Zoo" was proposed to help label one million images of galaxies collected by the Sloan Digital Sky Survey (SDSS) by posting images online and recruiting volunteers. 162 Larger optical telescopes, in operation or under construction, produce data several orders of magnitude higher than SDSS. Even with volunteers involved, there is no way to analyze the vast amount of data received. The advantages of ML are not limited to source-finding and galaxy classification. In fact, it has amuch wider range of applications. For example, CNN plays an important role in detecting and decoding gravitational wave signals in real time, reconstructing all parameters within 2 ms, while traditional algorithms take several days to accomplish the same task.163 Such DL systems have also been used to automatically generate alerts for transients and track asteroids and other fast-moving near-Earth objects, improving detection efficiency by several orders ofmagnitude. In addition, astrophysicists are exploring the use of neural networks to measure galaxy clusters and study the evolution of the Universe. In addition to the amazing speed, neural networks seem to have a deeper understanding of the data than expected and can recognize more complex patterns, indicating that the "machine" is evolving rather than just learning the characteristics of the input data.

AI IN CHEMISTRY

Chemistry plays an important "central" role in other sciences164 because it is the investigation of the structure and properties ofmatter, and identifies the chemical reactions that convert substances into to other substances. Accordingly, chemistry is a data-rich branch of science containing complex information resulting from centuries of experiments and, more recently, decades of computational analysis. This vast treasure trove of data is most apparent within the Chemical Abstract Services, which has collected more than 183 million unique organic and inorganic substances, including alloys, coordination compounds, minerals, mixtures, polymers, and salts, and is expanding by addition of thousands of additional new substances daily.165 The unlimited complexity in the variety of material compounds explains why chemistry research is still a labor-intensive task. The level of complexity and vast amounts of data within chemistry provides a prime opportunity to levels of theory used to describe the effects arising at different time and length scales, in the multi-scaling of chemical reactions.173 Many of the open challenges in computational chemistry can be solved by ML approaches, for example, solving Schrödinger's equation,174 developing atomistic175 or coarse graining176 potentials, constructing reaction coordinates,177 developing reaction kinetics models,178 and identifying key descriptors for computable properties.179 In addition to analytical chemistry and computational chemistry, several disciplines of chemistry have incorporated AI technology to chemical problems. We discuss the areas of organic chemistry, catalysis, and medical chemistry as examples of where ML has made a significant impact. Many examples exist in literature for other subfields of chemistry and AI will continue to demonstrate breakthroughs in a wide range of chemical applications.



AI helps to search through vast catalyst design spaces

Catalytic chemistry originates from catalyst technologies in the chemical industry for efficient and sustainable production of chemicals and fuels. Thus far, it is still a challenging endeavor to make novel heterogeneous catalysts with good performance (i.e., stable, active, and selective) because a catalyst's performance depends on many properties: composition, support, surface termination, particle size, particle morphology, atomic coordination environment, porous structure, and reactor during the reaction. The inherent complexity of catalysis makes discovering and developing catalysts with desired properties more dependent on intuition and experiment, which is costly and time consuming. AI technologies, such as ML, when combined with experimental and in silico high-throughput screening of combinatorial catalyst libraries, can aid catalyst discovery by helping to search through vast design spaces. With a well-defined structure and standardized data, including reaction results and in situ characterization results, the complex association between catalytic structure and catalytic performance will be revealed by AI.185,186 An accurate descriptor of the effect of molecules, molecular aggregation states, and molecular transport, on catalysts, could also be predicted. With this approach, researchers can build virtual laboratories to develop new catalysts and catalytic processes.

AI enables robotics capable of automating the synthesis of molecules

Organic chemistry studies the structure, property, and reaction of carbon- based molecules. The complexity of the chemical and reaction space, for a given property, presents an unlimited number of potential molecules that can be synthesized by chemists. Further complications are added when faced with the problems of how to synthesize a particular molecule, given that the process relies much on heuristics and laborious testing. Challenges have been addressed by researchers using AI. Given enough data, any properties of interest of a molecule can be predicted by mapping the molecular structure to the corresponding property using supervised learning, without resorting to physical laws. In addition to known molecules, new molecules can be designed by sampling the chemical space180 using methods, such as autoencoders and CNNs, with the molecules coded as sequences or graphs. Retrosynthesis, the planning of synthetic routes, which was once considered an art, has now become much simpler with the help of ML algorithms. The Chemetica system,181 for instance, is now capable of autonomous planning of synthetic routes that are subsequently proven to work in the laboratory. Once target molecules and the route of synthesis are determined, suitable reaction conditions can be predicted or optimized using ML techniques high enough exposure because of the already inherent complexity within living organisms. Moreover, toxicity is dependent on an array of other factors, including organism size, species, age, sex, genetics, diet, combination with other chemicals, overall health, and/or environmental context. Given the scale and complexity of toxicity problems, AI is likely to be the only realistic approach to meet regulatory body requirements for screening, prioritization, and risk assessment of chemicals (including mixtures), therefore revolutionizing the landscape in toxicology.187 In summary, AI is turning chemistry from a labor-intensive branch of science to a highly intelligent, standardized, and automated field, and much more can be achieved compared with the limitation of human labor.Underlying knowledge with new concepts, rules, and theories is expected to advance with the application of AI algorithms. A largeportion of new chemistry knowledge leading to significant breakthroughs isexpected to be generated from AI-based chemistry research in the decades to come.

CONCLUSIONS

This paper carries out a comprehensive survey on the development and application of AI across a broad range of fundamental sciences, including information science, mathematics, medical science, materials science, geoscience, life science, physics, and chemistry. Despite the fact that AI has beenpervasively used in a wide range of applications, there still exist ML security risks on data and ML models as attack targets during both training and execution phases. Firstly, since the performance of an ML system is highly dependent on the data used to train it, these input data are crucial for the security of the ML system. For instance, adversarial example attacks188 providing malicious input data often lead the ML system into making false judgments (predictions or categorizations) with small perturbations that are imperceptible to humans; data poisoning by intentionally manipulating raw, training, or testing data can result in a decrease in model accuracy or lead to other error-specific attack purposes. Secondly, ML model attacks include backdoor attacks on DL, CNN, and federated learning that manipulate the model's parameters directly, as well as model stealing attack, model inversion attack, and membership inference attack, which can steal the model parameters or leak the sensitive training data. While a number of defense techniques against these security threats have been proposed, new attack models that target ML systems are constantly emerging. Thus, it is necessary to address the problem ofML security and develop robust ML systems that remain effective under malicious attacks. Due to the data-driven character of theMLmethod, features of the training and testing data must be drawn from the same distribution, which is difficult to guarantee in practice. This is because, in practical application, the data source might be different from that in the training dataset. In addition, the data feature distribution may drift over time, which leads to a decline of the performance of the model. Moreover, if the model is trained with only new data, it will lead to catastrophic "forgetting" of the model, which means the model only remembers the new features and forgets the previously learned features. To solve this problem, more and more scholars pay attention on how to make the model have the ability of lifelong learning, that is, a change in the computing paradigm from "offline learning + online reasoning" to "online continuous learning," and thus give the model have the ability of lifelong learning, just like a human being.