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DATA SCIENCE



5 In-Demand Technical Skills for Data Scientists In 2022

"The field of data science is surging with the rising transformation in industries. For data scientists to be immaculate in their work, they have to market crucial programming languages and develop strong communication and interpersonal skills. The growing use of data has also risen the need for talented data scientists."

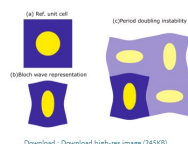
Source: Analytics Insight

Data science to Help Find the Most Appropriate Rehabilitation Methods for Osteoarthritis Patients

"A novel method, developed in collaboration between the Faculty of Information Technology and the Faculty of Sport and Health Sciences at the University of Jyväskylä, supports healthcare professionals in comparing and choosing the most preferred type of exercise based on an osteoarthritis patient's personalized needs.

The research will help us move towards more personalized treatment and therapy recommendations. Our method can help healthcare professionals to find the most appropriate rehabilitation method for each patient, which best meets the patient's needs, says Professor Kaisa

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Multiscale modeling of materials: Computing, data science, uncertainty and goal-oriented optimization

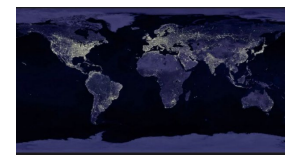
"The recent decades have seen various attempts at accelerating the process of developing materials targeted towards specific applications. The performance required for a particular application leads to the choice of a particular material system whose properties are optimized by manipulating its underlying microstructure through processing. The specific configuration of the structure is then designed by characterizing the material in detail, and using this characterization along with physical principles in system level simulations and optimization. These have been advanced by multiscale modeling of materials, high-throughput experimentations, materials data-bases, topology optimization and other ideas."

Source: Elsevier

When Quantum Computation Meets Data Science: Making Data Science Quantum

"Quantum computation and quantum information have attracted considerable attention on multiple frontiers of scientific fields ranging from physics to chemistry and engineering, as well as from computer science to mathematics

DATA SCIENCE



How Can Data Science Revolutionize Humanitarian Crises?

"Without 'orderly migration' and a renewed commitment to the Global Humanitarian Cooperation model, which you will learn about in his article, as well as good faith, equitable, and multilateral action by governments, we are doomed to repeat history over and over. As discussants to Purcell's piece, we hear from three very diverse voices in this advocacy sphere: the data science industry, the data science advocacy industry, and a close ally organization. It makes for a clear present-tense look at a past-tense overview.

After reflecting on what the past can teach practitioners, we highlight a discussion between IOM Director General António Vitorino and HDSR Editor-in-Chief Professor Xiao-Li Meng, who approach the issue of how improved data can be universally applied to the growing list of life-threatening human crises, originally posed by Purcell. Data science has permeated business, but the same cannot be said about global humanitarian issues. What more can we as data scientists do? What do those on the ground facing these humanitarian crises, day in and day out, need from us? Data science is a tool in the toolbox, what more can it do?"

Source: MIT Press

Miettinen from the University of Jyväskylä."

Source: University of Jyväskylä - Jyväskylän Yliopisto

Chemical data management: an open way forward

"Now, Smit, with Luc Patiny and Kevin Jablonka at EPFL, have published a perspective [in Nature Chemistry](#) presenting an open platform for the entire chemistry workflow: from the inception of a project to its publication.

The scientists envision the platform as "seamlessly" integrating three crucial steps: data collection, data processing, and data publication – all with minimal cost to researchers. The guiding principle is that data should be FAIR: easily findable, accessible, interoperable, and re-usable."

Source: Ecole Polytechnique Fédérale de Lausanne

DataX is funding eight new AI research projects across disciplines

"Eight new interdisciplinary research projects have won seed funding from Princeton University's Schmidt DataX Fund, marking the third round of grants undertaken by the fund since 2019. The fund, supported through a major gift from the Schmidt Futures Foundation, provides grants to explore using artificial intelligence and machine learning to accelerate discovery."

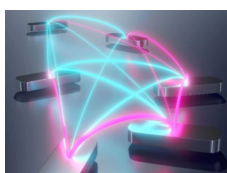
Source: Princeton University

Your Data Initiatives Can't Just Be for Data Scientists

"Regular people, those without "data" in their title, are central to all data-related work. Without buy-in and contributions from your company's rank and file, even the cleverest AI-derived model will sit idle and "data-driven decision-making" will just go around in circles. Conversely, costs go down and products get better when people help improve data quality, use small amounts of data to improve their team's processes, make better decisions, and contribute to larger data science and data monetization initiatives. Yet, recent research confirms that these people are missing from too many data programs, limiting the scale and impact of these efforts."

Source: Harvard Business News

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and statistics. Data science combines statistical methods, computational algorithms, and domain science information to extract knowledge and insights from big data, and to solve complex real-world problems. While it is well-known that quantum computation has the potential to revolutionize data science, much less has been said about the potential of data science to advance quantum computation."

Source: MIT Press

Data science and reinforcement learning for price forecasting and raw material procurement in petrochemical industry

"Petrochemical industry is one of the major sectors contributing to the world-wide economy and the digital transformation is urgent to enhance core competence. In general, ethylene, propylene and butadiene, which are associated with synthetic chemicals, are the main raw materials of this industry with around 70–80% cost structure. In particular, butadiene is one of the key materials for producing synthetic rubber and used for several daily commodities. However, the price of butadiene fluctuates along with the demand–supply mismatch or by the international economy and political events. This study proposes two-stage data science framework to predict the weekly price of butadiene and optimize the procurement decision."

Source: Elsevier

Data science roadmapping: An architectural framework for facilitating transformation towards a data-driven organization

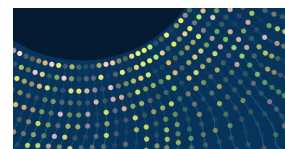
"Leveraging data science can enable businesses to exploit data for competitive advantage by generating valuable insights. However, many industries cannot effectively incorporate data science into their business processes, as there is no comprehensive approach that allows strategic planning for organization-wide data science efforts and data assets. Accordingly, this study explores the Data Science Roadmapping (DSR) to guide organizations in aligning their business strategies with data-related, technological, and organizational resources. The proposed approach is built on the widely adopted technology roadmapping framework and customizes its context, architecture, and process by synthesizing data science, big data, and data-driven organization literature. Based on industry collaborations, the framework

Data Science and Machine Learning (ML) Platforms Reviews and Ratings

"This market evaluates vendors of data science and machine-learning platforms. These are software products that data scientists use to help them develop and deploy their own data science and machine-learning solutions. More precisely, Gartner defines a data science and machine-learning platform as: A cohesive software application that offers a mixture of basic building blocks essential both for creating many kinds of data science solution and incorporating such solutions into business processes, surrounding infrastructure and products. Machine learning is a popular subset of data science that warrants specific attention when evaluating these platforms."

Source: Gartner

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Artificial Intelligence Index Report 2022

"Welcome to the fifth edition of the AI Index Report! The latest edition includes data from a broad set of academic, private, and nonprofit organizations as well as more self-collected data and original analysis than any previous editions, including an expanded technical performance chapter, a new survey of robotics researchers around the world, data on global AI legislation records in 25 countries, and a new chapter with an in-depth analysis of technical AI ethics metrics. The AI Index Report tracks, collates, distills, and visualizes data related to artificial intelligence. Its mission is to provide unbiased, rigorously vetted, and globally sourced data for policymakers, researchers, executives, journalists, and the general public to develop a more thorough and nuanced understanding of the complex field of AI. The report aims to be the world's most credible and authoritative source for data and insights about AI."

Source: Stanford University

2022 Report on the Global State of Artificial Intelligence

"From optimizing operations to driving R&D, enterprises are leveraging artificial intelligence (AI) to drive digital transformation and support business outcomes.

Printing Circuits on Nanomagnets Yields a New Breed of AI

"A rare form of matter known as "spin glass" may be opening up a new direction in artificial intelligence in which algorithms can be printed as physical hardware. Researchers at Los Alamos National Laboratory (LANL) have for the first time made an artificial spin glass consisting of nanomagnets arranged in a way that mimics a neural network. Theoretical models of spin glass have previously been widely used in complex systems, such as those describing brain function or stock market dynamics. In brief, spin glass is a magnetic state of matter that is characterized by randomness. The spin glass that the LANL researchers developed—published on 17 March in the journal *Nature Physics*—involves the magnets in the system finding a complex configuration of aligning and anti-aligning with each other to minimize energy use."

Source: IEEE Spectrum

New AI technique could lead to innovations in biomaterials

"The paper, titled "Coarse-grained molecular dynamics integrated with Convolutional Neural Network for comparing shapes of temperature sensitive bottlebrushes," details a method developed by the Deshmukh lab, including co-author and visiting scholar Samrendra Singh, that uses artificial intelligence to analyze the shape of important complex soft materials and predict their behaviors. It was published in *npj Computational Materials*, an open-access journal from Nature, and not only holds promise for enabling new discoveries in biomaterials, but highlights the growing importance of big data, artificial intelligence, and computational science in chemical engineering."

Source: Phys Org

'Mind-blowing': Ai-Da becomes first robot to paint like an artist

"Brush clamped firmly in bionic hand, Ai-Da's robotic arm moves slowly, dipping in to a paint palette then making slow, deliberate strokes across the paper in front of her.

This, according to Aidan Meller, the creator of the world's first ultra-realistic humanoid robot, Ai-Da, is "mind-blowing" and "groundbreaking" stuff.

In a small room at London's British Library, Ai-Da – assigned the she/her pronoun – has become the first robot to paint as artists have painted for centuries."

Source: The Guardian

provides a hybrid and agile methodology comprising the recommended steps."

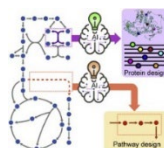
Source: Elsevier

Documentation Matters: Human-Centered AI System to Assist Data Science Code Documentation in Computational Notebooks

"Computational notebooks allow data scientists to express their ideas through a combination of code and documentation. However, data scientists often pay attention only to the code, and neglect creating or updating their documentation during quick iterations. Inspired by human documentation practices learned from 80 highly-voted Kaggle notebooks, we design and implement Themisto, an automated documentation generation system to explore how human-centered AI systems can support human data scientists in the machine learning code documentation scenario. Themisto facilitates the creation of documentation via three approaches: a deep-learning-based approach to generate documentation for source code, a query-based approach to retrieve online API documentation for source code, and a user prompt approach to nudge users to write documentation."

Source: ACM Digital Library

ARTIFICIAL INTELLIGENCE



Applications of artificial intelligence to enzyme and pathway design for metabolic engineering

"Metabolic engineering for developing industrial strains capable of overproducing bioproducts requires good understanding of cellular metabolism, including metabolic reactions and enzymes. However, metabolic pathways and enzymes involved are still unknown for many products of interest, which presents a key challenge in their biological production. This challenge can be partly overcome by constructing novel biosynthetic pathways through enzyme and pathway design approaches. With the increase in bio-big data, data-driven approaches using artificial intelligence (AI) techniques are allowing more advanced protein and pathway design. In this paper, we review recent studies on AI-aided protein engineering and design,

However, where are global organizations in this journey and what are their adoption drivers and restraints?

In this study, the analyst presents the key findings of a survey conducted among global enterprises on their state of adoption of AI. Respondents were drawn from senior IT decision makers across multiple verticals such as financial services, healthcare, retail, government, technology, and manufacturing.

The major themes explored in the survey include the current state of AI deployment, key organizational goals of AI implementation, the demand for specific AI-related technologies, and the main AI deployment models.

The study surveys technology vendors and service providers to obtain a view on AI priorities and help end users understand the benefits and the challenges of AI (as cited by global peers). In addition, the study gives readers an understanding of the prominent AI-related technologies that enterprises are adopting. It also offers insight into the main challenges enterprises face in their AI adoption journey."

Source: Business Wire

AI Adoption in the Enterprise 2022

"In December 2021 and January 2022, we asked recipients of our *Data and AI Newsletters* to participate in our annual survey on AI adoption. We were particularly interested in what, if anything, has changed since last year. Are companies farther along in AI adoption? Do they have working applications in production? Are they using tools like AutoML to generate models, and other tools to streamline AI deployment? We also wanted to get a sense of where AI is headed. The hype has clearly moved on to blockchains and NFTs. AI is in the news often enough, but the steady drumbeat of new advances and techniques has gotten a lot quieter. Compared to last year, significantly fewer people responded. That's probably a result of timing. This year's survey ran during the holiday season (December 8, 2021, to January 19, 2022, though we received very few responses in the new year); last year's ran from January 27, 2021, to February 12, 2021. Pandemic or not, holiday schedules no doubt limited the number of respondents."

Source: O'Reilly

Growth Opportunities in Cloud, Artificial Intelligence, and Edge Computing

"This edition of IT, Computing and Communications (ITCC) Technology Opportunity Engine (TOE) provides a

Stanford center uses AI and machine learning to expand data on women's and children's health, director says

"Stanford's Center for Artificial Intelligence in Medicine and Imaging (AIMI) is increasing engagement around the use of artificial intelligence (AI) and machine learning to build a better understanding of data on women's and children's health, according to AIMI Director and radiology professor Curt Langlotz.

Langlotz explained that, while AIMI initially focused on applying AI to medical imaging, it has since expanded its focus to applications of AI for other types of data, such as electronic health records.

Specifically, the center conducts "interdisciplinary machine learning research that optimizes how data of all forms are used to promote health," Langlotz said during a Monday event hosted by the Maternal and Child Health Research Institute (MCHRI). "And that interdisciplinary flavor is in our DNA."

Source: The Stanford Daily

Three former DeepMinders are developing A.I. to pick stocks and crypto

"They intend to use a technique known as reinforcement learning to train an AI system to buy and sell shares and make a profit. Reinforcement learning involves training an AI to achieve a particular goal (be that winning a game of chess or spotting a tumor on a mammogram) by giving it a reward each time.

Schmid said he's not concerned about regulators clamping down on the technology as other companies are already doing similar things. Indeed, EquiLibre Technologies will be competing with the likes of AI algorithmic stock picking products Candlestick and Yuyostox."

Source: CNBC

Announcing IBM z16: Real-time AI for Transaction Processing at Scale and Industry's First Quantum-Safe System

"IBM (NYSE: IBM) today unveiled IBM® z16™, IBM's next-generation system with an integrated on-chip AI accelerator—delivering latency-optimized inferencing. This innovation is designed to enable clients to analyze real-time transactions, at scale -- for mission-critical workloads such as credit card, healthcare and financial transactions. Building on IBM's history of security leadership, IBM z16 also is specifically designed to help protect against near-future

focusing on directed evolution that uses AI approaches to efficiently construct mutant libraries."

Source: Elsevier

Reconfigurable perovskite nickelate electronics for artificial intelligence

"Reconfigurable devices offer the ability to program electronic circuits on demand. In this work, we demonstrated on-demand creation of artificial neurons, synapses, and memory capacitors in post-fabricated perovskite NdNiO_3 devices that can be simply reconfigured for a specific purpose by single-shot electric pulses. The sensitivity of electronic properties of perovskite nickelates to the local distribution of hydrogen ions enabled these results. With experimental data from our memory capacitors, simulation results of a reservoir computing framework showed excellent performance for tasks such as digit recognition and classification of electrocardiogram heartbeat activity. Using our reconfigurable artificial neurons and synapses, simulated dynamic networks outperformed static network."

Source: Science

An explainable artificial intelligence approach for unsupervised fault detection and diagnosis in rotating machinery

"The monitoring of rotating machinery is an essential task in today's production processes. Currently, several machine learning and deep learning-based modules have achieved excellent results in fault detection and diagnosis. Nevertheless, to further increase user adoption and diffusion of such technologies, users and human experts must be provided with explanations and insights by the modules. Another issue is related, in most cases, with the unavailability of labeled historical data that makes the use of supervised models unfeasible. Therefore, a new approach for fault detection and diagnosis in rotating machinery is here proposed."

Source: Elsevier

A review of the hybrid artificial intelligence and optimization modelling of hydrological streamflow forecasting

"Ever since the first introduction of Artificial Intelligence into the field of hydrology, it has further generated immense interest in researching aspects for further improvements to hydrology. This can be seen in the rising number of related works published. This culminated further with

snapshot of the emerging ICT led innovations in Cloud, Artificial Intelligence and Edge Computing. This issue focuses on the application of information and communication technologies in alleviating the challenges faced across industry sectors in areas such as retail, industrial, BFSI, and automotive. ITCC TOE's mission is to investigate emerging wireless communication and computing technology areas including 3G, 4G, Wi-Fi, Bluetooth, Big Data, cloud computing, augmented reality, virtual reality, artificial intelligence, virtualization and the Internet of Things and their new applications; unearth new products and service offerings; highlight trends in the wireless networking, data management and computing spaces; provide updates on technology funding; evaluate intellectual property; follow technology transfer and solution deployment/integration; track development of standards and software; and report on legislative and policy issues and many more."

Source: Frost & Sullivan

Global Artificial Intelligence of Things (AIoT) in Telecommunications Growth Opportunities

"In this report, Frost & Sullivan examines the strategic position of telecommunication service providers (TSPs) in using artificial intelligence (AI) and the Internet of Things (IoT) to offer enterprises Artificial Intelligence of Things (AIoT) solutions. TSPs play a vital role in deploying enterprise AIoT solutions amid the increasing deployment of 5G networks, edge infrastructure capabilities, and location-based data at their disposal. Given their network and connectivity capabilities and AI and services focus, TSPs are in a unique position to monetize AIoT opportunities. They increasingly offer solutions by industry vertical as part of their AIoT focus. The report highlights TSPs' role as system integrators to provide value-added solutions and services to progress beyond connectivity and move up the value chain. Frost & Sullivan provides stakeholders insights by identifying AI growth drivers that will facilitate AIoT solutions deployment and opportunities in AI advisory and consulting services, edge infrastructure adoption, and building specific industry vertical solutions."

Source: Frost & Sullivan

Growth Opportunities in Artificial Intelligence, Low Code, Edge Computing, Cloud and IoT

threats that might be used to crack today's encryption technologies. IBM innovations, including the IBM z16, have formed the technology backbone of the global economy for decades. Today's modern IBM mainframe is central to hybrid cloud environments, valued by two thirds of the Fortune 100, 45 of the world's top 50 banks, 8 of the top 10 insurers, 7 of the top 10 global retailers and 8 out of the top 10 telcos as a highly secured platform for running their most mission critical workloads. For example, according to a recent IBM commissioned study by Celent "Operationalizing Fraud Prevention on IBM Z," IBM zSystems run 70% of global transactions, on a value basis."

Source: IBM

A.I. conquers bridge, one of the last games to fall to computer brains

"The Chess, Go, shogi, and poker are among the classic games that have, over the past two decades, fallen to A.I.'s dominance. Now you can add another to the list: bridge. Last week, in a special tournament in Paris, an A.I. system roundly defeated eight human world champions at the card game—or, at least an important phase of it—as my colleague Jonathan Vanian reported... The bridge-beating A.I. that Nukkai built, which it calls Nook, is different from the software that has in recent years bested humans at Go, shogi, and poker, as well as the complex video games Dota2 and Starcraft 2."

Source: Fortune

MACHINE LEARNING



Does this artificial intelligence think like a human?

"Now, researchers at MIT and IBM Research have created a method that enables a user to aggregate, sort, and rank these individual explanations to rapidly analyze a machine-learning model's behavior. Their technique, called Shared Interest, incorporates quantifiable metrics that compare how well a model's reasoning matches that of a human."

Shared Interest could help a user easily uncover concerning trends in a model's decision-making — for example, perhaps the model often becomes confused by distracting, irrelevant features, like background objects in photos. Aggregating these insights could help the user quickly and quantitatively determine whether a model is trustworthy and

the combination of pioneering optimization techniques. Who would have thought that the birds and the bees can offer advances in the mathematical sciences and so have the ants too? The ingenuity of humans is spelled out in the algorithms that mimic many natural activities, like pack hunting by the wolves! This review paper serves to broadcast more of the intriguing interest in newfound procedures in optimal forecasting."

Source: Elsevier

Leveraging artificial intelligence to improve people's planning strategies

"Human decision making is plagued by systematic errors that can have devastating consequences. Previous research has found that such errors can be partly prevented by teaching people decision strategies that would allow them to make better choices in specific situations. Three bottlenecks of this approach are our limited knowledge of effective decision strategies, the limited transfer of learning beyond the trained task, and the challenge of efficiently teaching good decision strategies to a large number of people. We introduce a general approach to solving these problems that leverages artificial intelligence to discover and teach optimal decision strategies. As a proof of concept, we developed an intelligent tutor that teaches people the automatically discovered optimal heuristic for environments where immediate rewards do not predict long-term outcomes."

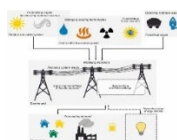
Source: PNAS

Provably Beneficial Artificial Intelligence

"As AI advances in capabilities and moves into the real world, its potential to benefit humanity seems limitless. Yet we see serious problems including racial and gender bias, manipulation by social media, and an arms race in lethal autonomous weapons. Looking further ahead, Alan Turing predicted the eventual loss of human control over machines that exceed human capabilities. I will argue that Turing was right to express concern but wrong to think that doom is inevitable. Instead, we need to develop a new kind of AI that is provably beneficial to humans."

Source: ACM Digital Library

MACHINE LEARNING



"This edition of IT, Computing and Communications (ITCC) Technology Opportunity Engine (TOE) provides a snapshot of the emerging ICT led innovations in Artificial Intelligence, Low Code, Edge Computing, Cloud and IoT. This issue focuses on the application of information and communication technologies in alleviating the challenges faced across industry sectors in areas such as retail, healthcare, Automotive, and manufacturing. ITCC TOE's mission is to investigate emerging wireless communication and computing technology areas including 3G, 4G, Wi-Fi, Bluetooth, Big Data, cloud computing, augmented reality, virtual reality, artificial intelligence, virtualization and the Internet of Things and their new applications; unearth new products and service offerings; highlight trends in the wireless networking, data management and computing spaces; provide updates on technology funding; evaluate intellectual property; follow technology transfer and solution deployment/integration; track development of standards and software; and report on legislative and policy issues and many more."

Source: Frost & Sullivan

ready to be deployed in a real-world situation."

Source: MIT

DataRobot's vision to democratize machine learning with no-code AI

"The growing digitization of nearly every aspect of our world and lives has created immense opportunities for the productive application of machine learning and data science. Organizations and institutions across the board are feeling the need to innovate and reinvent themselves by using artificial intelligence and putting their data to good use. And according to several surveys, data science is among the fastest-growing in-demand skills in different sectors. However, the growing demand for AI is hampered by the very low supply of data scientists and machine learning experts. Among the efforts to address this talent gap is the fast-evolving field of no-code AI, tools that make the creation and deployment of ML models accessible to organizations that don't have enough highly skilled data scientists and machine learning engineers."

Source: The Next Web

New Unique Machine Learning Tool Improves Experiences in Higher Education

"Explorance, a global leader in People Insight Solutions, announces today that BlueML, a one-of-a-kind machine learning platform, is now available for use by higher education institutions. BlueML swiftly transforms mass student qualitative feedback data into clear insights and actionable recommendations, improving teaching effectiveness and student success. The considerable amount of unstructured data gathered through course evaluations and other student surveys can make it difficult for institutions to process the responses and react to the feedback in a timely manner."

Source: Yahoo! Finance

Machine-learning method creates a learnable chemical grammar to build synthesizable monomers and polymers

"Chemical engineers and materials scientists are constantly looking for the next revolutionary material, chemical, and drug. The rise of machine-learning approaches is expediting the discovery process, which could otherwise take years. "Ideally, the goal is to train a machine-learning model on a few existing chemical samples and then allow it to produce as many manufacturable molecules of the same class as

Tackling Climate Change with Machine Learning

"Climate change is one of the greatest challenges facing humanity, and we, as machine learning (ML) experts, may wonder how we can help. Here we describe how ML can be a powerful tool in reducing greenhouse gas emissions and helping society adapt to a changing climate. From smart grids to disaster management, we identify high impact problems where existing gaps can be filled by ML, in collaboration with other fields. Our recommendations encompass exciting research questions as well as promising business opportunities. We call on the ML community to join the global effort against climate change."

Source: ACM Digital Library

PMLB v1.0: an open-source dataset collection for benchmarking machine learning methods

"Motivation

Novel machine learning and statistical modeling studies rely on standardized comparisons to existing methods using well-studied benchmark datasets. Few tools exist that provide rapid access to many of these datasets through a standardized, user-friendly interface that integrates well with popular data science workflows.

Results

This release of PMLB (Penn Machine Learning Benchmarks) provides the largest collection of diverse, public benchmark datasets for evaluating new machine learning and data science methods aggregated in one location. v1.0 introduces a number of critical improvements developed following discussions with the open-source community."

Source: Oxford Academic

Fusion-Based Supply Chain Collaboration Using Machine Learning Techniques

"Supply Chain Collaboration is the network of various entities that work cohesively to make up the entire process. The supply chain organizations' success is dependent on integration, teamwork, and the communication of information. Every day, supply chain and business players work in a dynamic setting. They must balance competing goals such as process robustness, risk reduction, vulnerability reduction, real financial risks, and resilience against just-in-time and cost-efficiency. Decision-making based on shared information in Supply Chain Collaboration constitutes the recital and competitiveness of the collective

possible, with predictable physical properties," says Wojciech Matusik, professor of electrical engineering and computer science at MIT. "If you have all these components, you can build new molecules with optimal properties, and you also know how to synthesize them. That's the overall vision that people in that space want to achieve."

Source: Phys Org

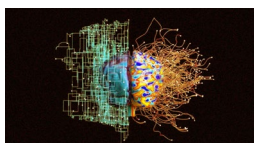
Researchers at MIT and IBM Propose an Efficient Machine Learning Method That Uses Graph Grammar to Generate New Molecules

"Chemical engineers and materials scientists are continuously looking for the following groundbreaking material, chemical, or medication. The emergence of machine-learning technologies has accelerated the discovery process, which may typically take years. Ideally, the objective is to train a machine-learning model on a few known chemical samples and then let it build as many manufacturable molecules of the same class with predictable physical attributes as feasible. You can develop new molecules with ideal characteristics if you have all of these components and the know-how to synthesize them.

However, current approaches need large datasets for training models. Many class-specific chemical databases only contain a few example compounds, restricting their capacity to generalize and construct biological molecules that might be generated in the real world."

Source: Mark Tech Post

DEEP LEARNING



What is Deep Learning? Significance of Deep Learning

"Deep learning computer algorithms go through the same procedure as a kid learning to recognize a dog. Each program in the hierarchy performs a nonlinear mapping on its input and then utilizes what it learns to generate a statistical model as output. Iterations are repeated until the result meets an acceptable degree of accuracy. The word deep was motivated by the number of processing layers that data must flow through.

The learning process in typical machine learning is monitored, and the programmer must be exceedingly detailed when instructing the computer on what sorts of things it should search for to determine if a

process. Supply Chain Collaboration has prompted companies to implement the perfect data analytics functions (e.g., data science, predictive analytics, and big data) to improve supply chain operations and, eventually, efficiency."

Source: Gachon University

Causality for Machine Learning

"Graphical causal inference as pioneered by Judea Pearl arose from research on artificial intelligence (AI), and for a long time had little connection to the field of machine learning. This chapter discusses where links have been and should be established, introduction key concepts along the way. It argues that the hard open problems of machine learning and AI are intrinsically related to causality, and explains how the field is beginning to understand them."

Source: ACM Digital Library

Interpretable machine learning: Fundamental principles and 10 grand challenges

"Interpretability in machine learning (ML) is crucial for high stakes decisions and troubleshooting. In this work, we provide fundamental principles for interpretable ML, and dispel common misunderstandings that dilute the importance of this crucial topic. We also identify 10 technical challenge areas in interpretable machine learning and provide history and background on each problem. Some of these problems are classically important, and some are recent problems that have arisen in the last few years. These problems are: (1) Optimizing sparse logical models such as decision trees; (2) Optimization of scoring systems; (3) Placing constraints into generalized additive models to encourage sparsity and better interpretability; (4) Modern case-based reasoning, including neural networks and matching for causal inference; (5) Complete supervised disentanglement of neural networks; (6) Complete or even partial unsupervised disentanglement of neural networks; (7) Dimensionality reduction for data visualization; (8) Machine learning models that can incorporate physics and other generative or causal constraints; (9) Characterization of the "Rashomon set" of good models; and (10) Interpretable reinforcement learning. This survey is suitable as a starting point for statisticians and computer scientists interested in working in interpretable machine learning."

Source: Project Euclid

DEEP LEARNING

picture includes or does not contain a dog. This is a time-consuming procedure known as feature extraction, and the computer's success rate is totally dependent on the programmer's ability to precisely specify a feature set for the dog. The benefit of deep learning is that the software creates the feature set without supervision. Unsupervised learning is not only quicker, but it is also more accurate in most cases."

Source: Analytics Insight

Deep learning algorithm shows accuracy in detecting glaucoma on fundus photographs

"Automated deep learning analysis of fundus photographs showed high diagnostic accuracy in determining primary open-angle glaucoma, with increased ability to detect glaucoma earlier than human readers.

A deep learning (DL) algorithm was trained, validated and tested on the fundus stereophotographs of participants enrolled in the Ocular Hypertension Treatment Study (OHTS), a randomized clinical trial evaluating the safety and efficacy of IOP-lowering medications in preventing progression from ocular hypertension to primary open-angle glaucoma (POAG). Assessment of optic disc and visual field changes in the OHTS was performed by two reading centers and a masked committee of glaucoma specialists, "a demanding, laborious and complicated task," according to the authors."

Source: Heaio

NEURAL NETWORK



An optimized solution for face recognition

"Dobs, who is now a research group leader at Justus Liebig University Giessen in Germany, assembled hundreds of thousands of images with which to train a deep neural network in face and object recognition. The collection included the faces of more than 1,700 different people and hundreds of different kinds of objects, from chairs to cheeseburgers. All of these were presented to the network, with no clues about which was which. "We never told the system that some of those are faces, and some of those are objects. So it's basically just one big task," Dobs says. "It needs to recognize a face identity, as well as a bike or a pen."

As the program learned to identify the objects and faces, it organized itself into an information-processing



Review on deep learning techniques for marine object recognition: Architectures and algorithms

"Due to the rapid development of deep learning techniques, numerous frameworks including convolutional neural networks (CNNs), deep belief networks (DBNs) and auto-encoder (AE), etc., have been established. In this context, advances in marine object recognition have been dramatically boosted, especially in the past decade. In this paper, we exclusively focus on an intensive review on deep-learning-based object recognition for both surface and underwater targets. To facilitate a comprehensive review, key concepts and typical architectures are firstly summarized in a unified framework.

Accordingly, popular/benchmark datasets for marine object recognition are thoroughly collected and deep learning methodologies are comprehensively analyzed with intensive comparisons."

Source: Elsevier

Big data analysis of the Internet of Things in the digital twins of smart city based on deep learning

"The study aims to conduct big data analysis (BDA) on the massive data generated in the smart city Internet of things (IoT), make the smart city change to the direction of fine governance and efficient and safe data processing. Aiming at the multi-source data collected in the smart city, the study introduces the deep learning (DL) algorithm while using BDA, and puts forward the distributed parallelism strategy of convolutional neural network (CNN). Meantime, the digital twins (DTs) and multi-hop transmission technology are introduced to construct the smart city DTs multi-hop transmission IoT-BDA system based on DL, and further simulate and analyze the performance of the system. The results reveal that in the energy efficiency analysis of model data transmission, the energy efficiency first increases and then decrease as the minimum energy collected increase."

Source: Elsevier

Using deep learning to annotate the protein universe

"Understanding the relationship between amino acid sequence and protein function is a long-standing

network with that included units specifically dedicated to face recognition. Like the brain, this specialization occurred during the later stages of image processing. In both the brain and the artificial network, early steps in facial recognition involve more general vision processing machinery, and final stages rely on face-dedicated components."

Source: MIT

Rational neural network advances machine-human discovery

"In the new and growing field of partial differential equation (PDE) learning, mathematicians collect data from natural systems and then use trained computer neural networks in order to try to derive underlying mathematical equations. In a new paper, Townsend, together with co-authors Nicolas Boullé of the University of Oxford and Christopher Earls, professor of civil and environmental engineering in the College of Engineering, advance PDE learning with a novel "rational" neural network, which reveals its findings in a manner that mathematicians can understand: through Green's functions – a right inverse of a differential equation in calculus. This machine-human partnership is a step toward the day when deep learning will enhance scientific exploration of natural phenomena such as weather systems, climate change, fluid dynamics, genetics and more. "Data-Driven Discovery of Green's Functions With Human-Understandable Deep Learning" was published in Scientific Reports, Nature on March 22."

Source: Cornell University

MEDICAL TECHNOLOGY



Can A.I.-Driven Voice Analysis Help Identify Mental Disorders?

"Imagine a test as quick and easy as having your temperature taken or your blood pressure measured that could reliably identify an anxiety disorder or predict an impending depressive relapse.

Health care providers have many tools to gauge a patient's physical condition, yet no reliable biomarkers — objective indicators of medical states observed from outside the patient — for assessing mental health. But some artificial intelligence researchers now believe that the sound of your voice might be the key to understanding your mental state — and A.I. is perfectly suited to detect

challenge with far-reaching scientific and translational implications. State-of-the-art alignment-based techniques cannot predict function for one-third of microbial protein sequences, hampering our ability to exploit data from diverse organisms. Here, we train deep learning models to accurately predict functional annotations for unaligned amino acid sequences across rigorous benchmark assessments built from the 17,929 families of the protein families database Pfam. The models infer known patterns of evolutionary substitutions and learn representations that accurately cluster sequences from unseen families. Combining deep models with existing methods significantly improves remote homology detection, suggesting that the deep models learn complementary information. This approach extends the coverage of Pfam by >9.5%, exceeding additions made over the last decade, and predicts function for 360 human reference proteome proteins with no previous Pfam annotation."

Source: Nature

A review of speaker diarization: Recent advances with deep learning

"Speaker diarization is a task to label audio or video recordings with classes that correspond to speaker identity, or in short, a task to identify "who spoke when". In the early years, speaker diarization algorithms were developed for speech recognition on multispeaker audio recordings to enable speaker adaptive processing. These algorithms also gained their own value as a standalone application over time to provide speaker-specific meta-information for downstream tasks such as audio retrieval. More recently, with the emergence of deep learning technology, which has driven revolutionary changes in research and practices across speech application domains, rapid advancements have been made for speaker diarization. In this paper, we review not only the historical development of speaker diarization technology but also the recent advancements in neural speaker diarization approaches."

Source: Elsevier

Error estimates for DeepONets: a deep learning framework in infinite dimensions

"DeepONets have recently been proposed as a framework for learning nonlinear operators mapping between infinite-dimensional Banach spaces. We analyze DeepONets and prove estimates on the resulting

such changes, which are difficult, if not impossible, to perceive otherwise. The result is a set of apps and online tools designed to track your mental status, as well as programs that deliver real-time mental health assessments to telehealth and call-center providers."

Source: New York Times

First autonomous X-ray-analyzing AI is cleared in the EU

"An artificial intelligence tool that reads chest X-rays without oversight from a radiologist got regulatory clearance in the European Union last week — a first for a fully autonomous medical imaging AI, the company, called Oxipit, said in a statement. It's a big milestone for AI and likely to be contentious, as radiologists have spent the last few years pushing back on efforts to fully automate parts of their job. The tool, called ChestLink, scans chest X-rays and automatically sends patient reports on those that it sees as totally healthy, with no abnormalities. Any images that the tool flags as having a potential problem are sent to a radiologist for review. Most X-rays in primary care don't have any problems, so automating the process for those scans could cut down on radiologists' workloads, the Oxipit said in informational materials."

Source: The Verge

Researchers identify new medicines using interpretable deep learning predictions

"An important aspect of drug discovery involves determining how well a drug binds to its target (protein) molecule. Typically, this step involves aligning a 3D structure of a drug and its target protein at various configurations in a process called "docking." Preferred binding sites are then discovered by running docking simulations repeatedly with multiple drug candidates for a particular target molecule. Typically, owing to the vast number of likely candidates for potential drug-target interactions, deep learning models are used to carry out such simulations. However, a problem with using such models is the difficulty in interpreting their predictions. While deep learning certainly makes for a speedy drug discovery, it is little more than a black box. Additionally, docking simulations cannot be used to develop drugs for novel targets that have no known 3D complex with an interacting drug."

Source: Medical Express

Artificial intelligence may improve diabetes diagnosis

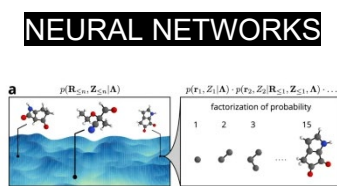
approximation and generalization errors. In particular, we extend the universal approximation property of DeepONets to include measurable mappings in non-compact spaces. By a decomposition of the error into encoding, approximation and reconstruction errors, we prove both lower and upper bounds on the total error, relating it to the spectral decay properties of the covariance operators, associated with the underlying measures. We derive almost optimal error bounds with very general affine reconstructors and with random sensor locations as well as bounds on the generalization error, using covering number arguments."

Source: Oxford Academic

Towards automatic threat detection: A survey of advances of deep learning within X-ray security imaging

"X-ray security screening is widely used to maintain aviation/transport security, and its significance poses a particular interest in automated screening systems. This paper aims to review computerised X-ray security imaging algorithms by taxonomising the field into conventional machine learning and contemporary deep learning applications. The first part briefly discusses the classical machine learning approaches utilised within X-ray security imaging, while the latter part thoroughly investigates the use of modern deep learning algorithms. The proposed taxonomy sub-categorises the use of deep learning approaches into supervised and unsupervised learning, with a particular focus on object classification, detection, segmentation and anomaly detection tasks."

Source: Elsevier



Inverse design of 3d molecular structures with conditional generative neural networks

"The rational design of molecules with desired properties is a long-standing challenge in chemistry. Generative neural networks have emerged as a powerful approach to sample novel molecules from a learned distribution. Here, we propose a conditional generative neural network for 3d molecular structures with specified chemical and structural properties. This approach is agnostic to chemical bonding and enables targeted sampling of novel molecules from conditional distributions, even in

"Using a fully-automated artificial intelligence (AI) deep learning model, researchers were able to identify early signs of type 2 diabetes on abdominal CT scans, according to a new study published in the journal *Radiology*.

Type 2 diabetes affects approximately 13% of all U.S. adults and an additional 34.5% of adults meet the criteria for prediabetes. Due to the slow onset of symptoms, it is important to diagnose the disease in its early stages. Some cases of prediabetes can last up to 8 years and an earlier diagnosis will allow patients to make lifestyle changes to alter the progression of the disease."

Source: EurekAlert

domains where reference calculations are sparse. We demonstrate the utility of our method for inverse design by generating molecules with specified motifs or composition, discovering particularly stable molecules, and jointly targeting multiple electronic properties beyond the training regime."

Source: Nature Communications

Physics-informed neural networks (PINNs) for fluid mechanics: a review

"Despite the significant progress over the last 50 years in simulating flow problems using numerical discretization of the Navier-Stokes equations (NSE), we still cannot incorporate seamlessly noisy data into existing algorithms, mesh-generation is complex, and we cannot tackle high-dimensional problems governed by parametrized NSE. Moreover, solving inverse flow problems is often prohibitively expensive and requires complex and expensive formulations and new computer codes. Here, we review flow physics-informed learning, integrating seamlessly data and mathematical models, and implement them using physics-informed neural networks (PINNs). We demonstrate the effectiveness of PINNs for inverse problems related to three-dimensional wake flows, supersonic flows, and biomedical flows."

Source: Springer Link

Analyses of internal structures and defects in materials using physics-informed neural networks

"Characterizing internal structures and defects in materials is a challenging task, often requiring solutions to inverse problems with unknown topology, geometry, material properties, and nonlinear deformation. Here, we present a general framework based on physics-informed neural networks for identifying unknown geometric and material parameters. By using a mesh-free method, we parameterize the geometry of the material using a differentiable and trainable method that can identify multiple structural features. We validate this approach for materials with internal voids/inclusions using constitutive models that encompass the spectrum of linear elasticity, hyperelasticity, and plasticity. We predict the size, shape, and location of the internal void/inclusion as well as the elastic modulus of the inclusion."

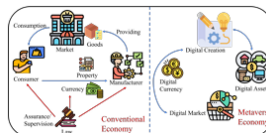
Source: Science Advances

Quantum convolutional neural networks for high energy physics data analysis

"This paper presents a quantum convolutional neural network (QCNN) for the classification of high energy physics events. The proposed model is tested using a simulated dataset from the Deep Underground Neutrino Experiment. The proposed quantum architecture demonstrates an advantage of learning faster than the classical convolutional neural networks (CNNs) under a similar number of parameters. In addition to the faster convergence, the QCNN achieves a greater test accuracy compared to CNNs. Based on our results from numerical simulations, it is a promising direction to apply QCNN and other quantum machine learning models to high energy physics and other scientific fields."

Source: APS Physics

METaverse



Fusing Blockchain and AI with Metaverse: A Survey

"Metaverse as the latest buzzword has attracted great attention from both industry and academia. Metaverse seamlessly integrates the real world with the virtual world and allows avatars to carry out rich activities including creation, display, entertainment, social networking, and trading. Thus, it is promising to build an exciting digital world and to transform a better physical world through the exploration of the metaverse. In this survey, we dive into the metaverse by discussing how Blockchain and Artificial Intelligence (AI) fuse with it through investigating the state-of-the-art studies across the metaverse components, digital currencies, AI applications in the virtual world, and blockchain-empowered technologies. Further exploitation and interdisciplinary research on the fusion of AI and Blockchain towards metaverse will definitely require collaboration from both academia and industries. We wish that our survey can help researchers, engineers, and educators build an open, fair, and rational future metaverse."

Source: Cornell University

Overview: Technology Roadmap of the Future Trend of Metaverse based on IoT, Blockchain, AI Technique, and

Medical Domain Metaverse Activity

"Metaverse is defined as a collection of technology gadgets and metaverse connected to IoT, Blockchain, Artificial Intelligence, and all the other tech industries including the medical area. IoT and Metaverse are the digital twins, Metaverse is using maximum IoT devices in their virtual workstation. This data has a unique identifying tag and is used as traceable data in the blockchain-based Metaverse. In the Metaverse, such data is becoming a valuable resource for artificial intelligence. Metaverse uses artificial intelligence and blockchain technology to build a digital virtual world where you can safely and freely engage in social and economic activities that transcend the limits of the real world, and the application of these latest technologies will be expedited. In this paper, we are going to describe what technologies metaverse is using and metaverse potentiality in medical healthcare."

Source: IEEE Xplore

Artificial Intelligence for the Metaverse: A Survey

"Along with the massive growth of the Internet from the 1990s until now, various innovative technologies have been created to bring users breathtaking experiences with more virtual interactions in cyberspace. Many virtual environments with thousands of services and applications, from social networks to virtual gaming worlds, have been developed with immersive experience and digital transformation, but most are incoherent instead of being integrated into a platform. In this context, metaverse, a term formed by combining meta and universe, has been introduced as a shared virtual world that is fueled by many emerging technologies, such as fifth-generation networks and beyond, virtual reality, and artificial intelligence (AI). Among such technologies, AI has shown the great importance of processing big data to enhance immersive experience and enable human-like intelligence of virtual agents. In this survey, we make a beneficial effort to explore the role of AI in the foundation and development of the metaverse."

Source: Cornell University