

# TOPICAL REPORT

## ARTIFICIAL INTELLIGENCE & DATA SCIENCE

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### DATA SCIENCE



#### How CI/CD is different for data science

"Agile programming is the most-used methodology that enables development teams to release their software into production, frequently to gather feedback and refine the underlying requirements. For agile to work in practice, however, processes are needed that allow the revised application to be built and released into production automatically—generally known as continuous integration/continuous deployment, or CI/CD. CI/CD enables software teams to build complex applications without running the risk of missing the initial requirements by regularly involving the actual users and iteratively incorporating their feedback.

Data science faces similar challenges. Although the risk of data science teams missing the initial requirements is less of a threat right now (this will change in the coming decade), the challenge inherent in automatically deploying data science into production brings many data science projects to a grinding halt. First, IT too often needs to be involved to put anything into the production system. Second, validation is typically an unspecified, manual task (if it even exists). And third, updating a production data science process reliably is often so

### DATA SCIENCE



#### 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 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. Yet because the stochasticity of quantum physics renders quantum computation random, data science can play an important role in the development of quantum computation and quantum information. This article gives an overview of quantum computation and promotes interplay between quantum science and data science."

Source: MIT Press

**A practical, effective calculation of gamma**

### DATA SCIENCE



#### 20 Data Engineering Platforms & Skills Needed in 2022

"Data engineering is overtaking "data science" as the hot skillset of the 2020s. Companies are actively seeking people to collect data and load it into pipelines for the rest of the data science team to clean and organize. Without this data, there would be no data science team – and more importantly, no data to gather important insights from. As we look to the year ahead, we scoured over 18,000 data engineering jobs to find what companies are looking for. These data engineering platforms and skills are good to learn for anyone looking for a job in data engineering, or for anyone already practicing who's looking to round out their skillset."

Source: Open Data Science

### ARTIFICIAL INTELLIGENCE



#### Artificial Intelligence for Human Resources Toolkit Helps Organizations Overcome Implementation Challenges

"Artificial intelligence (AI) has gained considerable attention and

difficult, it's treated as an entirely new project."

Source: InfoWorld

## Big Data in Life Sciences – Why 'doing things the old way' is the Biggest Barrier to Progress

"In this special guest feature, Zachary Pitluk, Ph.D., Vice President of Life Sciences and Healthcare at Paradigm4, highlights how real insight comes, not from data collection, but from intelligent data curation, computation, and application. Zachary has worked in sales and marketing for 23 years, from being a pharmaceutical representative for BMS to management roles in Life Science technology companies. Since 2003, his positions have included VP of Business Development at Gene Network Sciences and Chief Commercial officer at Proveris Scientific. Zach has held academic positions at Yale University Department of Molecular Biophysics and Biochemistry: Associate Research Scientist, Postdoctoral Fellow and Graduate Student, and has been named as co-inventor on numerous patents."

Source: Inside Big Data

## ARTIFICIAL INTELLIGENCE



## A New Method to Make AI-Generated Voices More Expressive

"Researchers have found a way to make AI-generated voices, such as digital personal assistants, more expressive, with a minimum amount of training. The method, which translates text to speech, can also be applied to voices that were never part of the system's training set.

The team of computer scientists and electrical engineers from the University of California San Diego presented their work at the ACML 2021 conference, which took place online recently.

In addition to personal assistants for smartphones, homes and cars, the method could help improve voice-overs in animated movies, automatic translation of speech in multiple languages—and more. The method could also help create personalized speech interfaces that empower individuals who have lost the ability to speak, similar to the computerized voice that Stephen Hawking used to communicate, but far more expressive."

Source: UC San Diego

## difference distributions with open data science tools

"At present, there is still no officially accepted and extensively verified implementation of computing the gamma difference distribution allowing unequal shape parameters. We explore four computational ways of the gamma difference distribution with different shape parameters resulting from time series kriging, a forecasting approach based on the best linear unbiased prediction and linear mixed models. The results of our numerical study, with emphasis on using open data science tools, demonstrate that our computational algorithm implemented in high-performance Python (with Numba) is exponentially fast, highly accurate and very reliable. It combines numerical inversion of the characteristic function and the trapezoidal rule with the double exponential oscillatory transformation (DE quadrature). At the double 53-bit precision, our open tool outperformed the speed of the analytical computation based on Tricomi's  $U(a,b,z)$  function in CAS software (commercial Mathematica, open SageMath) by 1.5–2 order."

Source: Taylor & Francis Online

## Big Data and Disinformation: Algorithm Mapping for Fact Checking and Artificial Intelligence

"This chapter looks at the intricate relationship between journalism and mathematics (big data, algorithms, data mining) as a tool to verify information and fight disinformation. The first section focuses on the relationship current students have with techniques such as big data or artificial intelligence and their ideas on applying them to their profession. The second section maps which universities and researchers in the world are looking into that relationship, how they approach it and where they publish their results. A relevant result is the presence of engineers in those studies, as well as Asian-origin researchers. Finally, we present results that show the increasingly close relationship between different disciplines such as computational linguistics, artificial intelligence and big data to solve the challenge of fake news and disinformation."

Source: Springer Link

## How Can Data Science Revolutionize Humanitarian Crises?

"As co-editors of the special theme on migration for Harvard Data Science Review (HDSR), we identified an opportunity to incorporate both

excitement in recent years. Broadly defined as the effort to program computers to take on human-like cognitive processes, the recent prominence of AI is closely tied to the success of machine learning (ML), an approach to developing AI systems using real-world examples. The ML approach is applicable to a surprisingly wide variety of use cases; therefore, there is a proliferation of AI-based tools in every sector of the economy and of life. The field of human resources (HR) is no exception. Indeed, by one count there are over 250 different commercial AI-based HR tools available. These tools offer a lot of promise and excitement. Beyond their ability to process information quickly, these tools have the potential to improve HR processes, leading to better decisions and outcomes. Their variety reflects the creativity and innovation spurred by recent advancements in AI, as their creators seek to both tackle long-standing challenges in HR and expand capacities into new realms. At the same time, this proliferation and variety of tools creates a confusing landscape to navigate, especially because most HR professionals do not feel that they have the technical expertise required to evaluate these tools. The first goal of this toolkit, therefore, is to equip HR professionals with a basic understanding of AI to assist them in their efforts to assess AI-based tools."

Source: World Economic Forum

## The state of AI in 2021

"The results of our latest McKinsey Global Survey on AI indicate that AI adoption continues to grow and that the benefits remain significant—though in the COVID-19 pandemic's first year, they were felt more strongly on the cost-savings front than the top line. As AI's use in business becomes more common, the tools and best practices to make the most out of AI have also become more sophisticated.

We looked at the practices of the companies seeing the biggest earnings boost from AI and found that they are not only following more of both the core and advanced practices, including machine-learning operations (MLOps), that underpin success but also spending more efficiently on AI and taking more advantage of cloud technologies. Additionally, they are more likely than other organizations to engage in a range of activities to mitigate their AI-related risks—an area that continues to be a shortcoming for many companies' AI efforts."

Source: McKinsey & Company

## Artificial intelligence system rapidly predicts how two proteins will attach

"Antibodies, small proteins produced by the immune system, can attach to specific parts of a virus to neutralize it. As scientists continue to battle SARS-CoV-2, the virus that causes Covid-19, one possible weapon is a synthetic antibody that binds with the virus' spike proteins to prevent the virus from entering a human cell..."

To streamline the process, MIT researchers created a machine-learning model that can directly predict the complex that will form when two proteins bind together. Their technique is between 80 and 500 times faster than state-of-the-art software methods, and often predicts protein structures that are closer to actual structures that have been observed experimentally."

Source: MIT

## Technique Smooths Path for 'Federated Learning' AI Training in Wireless Devices

"Federated learning is a form of machine learning involving multiple devices, called clients. Each of the clients is trained using different data and develops its own model for performing a specific task. The clients then send their models to a centralized server. The centralized server draws on each of those models to create a hybrid model, which performs better than any of the other models on their own. The central server then sends this hybrid model back to each of the clients. The entire process is then repeated, with each iteration leading to model updates that ultimately improve the system's performance."

Source: NC State University

## Technique Improves AI Ability to Understand 3D Space Using 2D Images

"The World Robotics report shows that Europe is the region with the highest robot density globally, with an average value of 114 units per 10,000 employees in the manufacturing industry. For more facts about robots watch IFR's video news about Europe in one minute."

Source: North Carolina State University

## Studying the Big Bang with Artificial Intelligence

"It could hardly be more complicated: tiny particles whir around wildly with extremely high energy, countless interactions occur in the tangled mess of quantum particles, and this results in a state of matter known as "quark-gluon plasma". Immediately after the Big

an academic and industry exploration of multiple aspects of forced displacement and world migration. Diverse perspectives evaluate migration in its current context, as well as lessons from previous crises, and how both can impact how we address concerns in the future. We recall the highlights of the HDSR World Migration and Displacement Symposium in the spring of 2021, and bring in multiple ideas and outcomes from this symposium from leaders and experts on all sides of the working fence: academic, non-governmental organization, and industry. We hope this issue will illuminate some of the enormous struggles, as well as the bright and enduring future, of forced displacement and migration.

In spring 2020, when COVID-19 hit the world like a firestorm, a vulnerable, yet highly resilient group of people were left in dire straits."

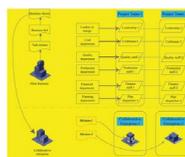
Source: MIT Press

## Data Science Toolkit: An all-in-one python library to help researchers and practitioners in implementing data science-related algorithms with less effort

"Data Science Toolkit (DST) is a python library built as a wrapper layer on top of several libraries to increase the abstraction level of the code, making its users more efficient and productive. The current version is widely used in our ongoing research activities that focus on optimizing agricultural management practices using artificial intelligence. DST adopts an object-oriented approach in implementing data science algorithms and is therefore composed of multiple classes such as the DataFrame class that adds additional functionalities to the standard pandas dataframe and the Model class that facilitates the building, training, and evaluation of machine learning models."

Source: Research Gate

## ARTIFICIAL INTELLIGENCE



## Modeling of an Enterprise Knowledge Management System Based on Artificial Intelligence

"Enterprise knowledge management research is required to improve the enterprise content management system and knowledge management theory. A general model of

## 2021 Artificial Intelligence and Automated Systems Annual Legal Review

"2021 was a busy year for policy proposals and lawmaking related to artificial intelligence ("AI") and automated technologies. The OECD identified 700 AI policy initiatives in 60 countries, and many domestic legal frameworks are taking shape. With the new Artificial Intelligence Act, which is expected to be finalized in 2022, it is likely that high-risk AI systems will be explicitly and comprehensively regulated in the EU. While there have been various AI legislative proposals introduced in Congress, the United States has not embraced a comprehensive approach to AI regulation as proposed by the European Commission, instead focusing on defense and infrastructure investment to harness the growth of AI.

Nonetheless—mirroring recent developments in data privacy laws—there are some tentative signs of convergence in US and European policymaking, emphasizing a risk-based approach to regulation and a growing focus on ethics and "trustworthy" AI, as well as enforcement avenues for consumers. In the U.S., President Biden's administration announced the development of an "AI bill of rights." Moreover, the U.S. Federal Trade Commission ("FTC") has signaled a particular zeal in regulating consumer products and services involving automated technologies and large data volumes, and appears poised to ramp up both rulemaking and enforcement activity in the coming year. Additionally, the new California Privacy Protection Agency will likely be charged with issuing regulations governing AI by 2023, which can be expected to have far-reaching impact. Finally, governance principles and technical standards for ensuring trustworthy AI and ML are beginning to emerge, although it remains to be seen to what extent global regulators will reach consensus on key benchmarks across national borders."

Source: Gibson Dunn

## Growth Opportunities in Quantum Computing, Virtual Reality, Artificial Intelligence, and 5G

"This edition of IT, Computing and Communications (ITCC) Technology Opportunity Engine (TOE) provides a snapshot of the ICT led innovations in quantum computing, virtual reality, artificial intelligence, and 5G. This issue focuses on the application of information and communication technologies in alleviating the

Bang, the entire universe was in this state; today it is produced by high-energy atomic nucleus collisions, for example at CERN.

Such processes can only be studied using high-performance computers and highly complex computer simulations whose results are difficult to evaluate. Therefore, using artificial intelligence or machine learning for this purpose seems like an obvious idea. Ordinary machine-learning algorithms, however, are not suitable for this task. The mathematical properties of particle physics require a very special structure of neural networks. At TU Wien (Vienna), it has now been shown how neural networks can be successfully used for these challenging tasks in particle physics."

Source: TU Wien

## Can AI Predict Thermal Comfort from The Layout of a Room?

"In a recent study published in the Journal of Building Engineering, a team of scientists—including Dr Cheng Zhang and Dr Bing Chen, both from Xi'an Jiaotong-Liverpool University's Design School—sought to address this knowledge gap.

"Our research set out to determine exactly how we can map the thermal comfort of different areas of a room, and how factors such as sunlight exposure, windows, and HVAC positioning affect each area," explains Dr Zhang. "To this end, we developed an artificial neural network (ANN)-based system to predict personal thermal comfort based on these factors.""

Source: Xi'an Jiaotong Liverpool University

## Best practices for developing governable AI

"Building and deploying strong, robust artificial intelligence (AI) and machine learning (ML) models is complex and challenging work. If you are like many data science and machine learning leaders that I have spoken to lately, you are having conversations with other teams about the governance of your systems.

It's hard to do that and do your job of getting models into production. So let's talk about what you can do as a technical organization to make AI governance easier both for your team and your business partners, who are key stakeholders in the governance process."

Source: InfoWorld

## MACHINE LEARNING

knowledge integration is developed based on the concept of multi-view modelling, starting with the necessity for knowledge integration and application in the networked manufacturing process of complex products. This paper used social exchange theory to explain chain transmission's online knowledge transfer process and analysed the related influencing factors. In addition, the key technologies that need to be solved to achieve knowledge integration, including the integration of distributed heterogeneous knowledge among enterprises, correlation integration, and integration of knowledge and manufacturing processes, were pointed out. The fuzzy theory was used to establish the knowledge extraction mechanism and reference model library from the project model to the dedicated reference model."

Source: Taylor & Francis Online

## Solving Conformal Field Theories with Artificial Intelligence

"In this Letter, we deploy for the first time reinforcement-learning algorithms in the context of the conformal-bootstrap program to obtain numerical solutions of conformal field theories (CFTs). As an illustration, we use a soft actor-critic algorithm and find approximate solutions to the truncated crossing equations of two-dimensional CFTs, successfully identifying well-known theories like the 2D Ising model and the 2D CFT of a compactified scalar. Our methods can perform efficient high-dimensional searches that can be used to study arbitrary (unitary or nonunitary) CFTs in any spacetime dimension."

Source: APS Physics

## Effects of Using Artificial Intelligence on Interpersonal Perceptions of Job Applicants

"Text-based artificial intelligence (AI) systems are increasingly integrated into a host of interpersonal domains. Although decision-making and person perception in hiring and employment opportunities have been an area of psychological interest for many years, only recently have scholars begun to investigate the role that AI plays in this context. To better understand the impact of AI in employment-related contexts, we conducted two experiments investigating how the use of AI by applicants influences their job opportunities. In our preregistered Study 1, we examined how a prospective job applicants' use of AI, as well as their language status (native English speaker or non-native English speaker), influenced

challenges faced across industry sectors in areas such as retail, healthcare, BFSI, 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

## Global Artificial Intelligence in Supply Chain Management Growth Opportunities

"Artificial intelligence (AI) and cognitive technologies are becoming a critical element of supply chain management (SCM) solutions as they evolve from point to integrated solutions. AI plays a vital role in making SCM more agile, transparent, and customer-oriented.

In this report, Frost & Sullivan examines the importance of AI in transforming SCM, identifies critical challenges in SCM—especially in the post-COVID-19 era—and recognizes AI and other cognitive technologies as a natural fit for SCM. Our analysis shows that AI and other emerging cognitive technologies will be the key enablers in developing new supply chain models that allow companies to reach customers more effectively. The report details SCM market trends and studies AI's impact in each SCM sub-function, from procurement to customer support services. Most importantly, we offer stakeholders insights into crucial growth opportunities that will shape the industry over the next 2–3 years."

Source: Frost & Sullivan



## Towards Greener Smart Cities with Machine Learning-Based "Sleep Schedules"

"While cellular networks are the foundation of smart cities, they consume a lot of energy, enhancing global warming. Putting base stations (BSs) with low traffic to sleep saves energy but also reduces traffic prediction accuracy. In a new study, researchers from Japan address this trade-off using machine learning technique to switch off BSs based on their contribution to prediction accuracy. The new scheme reduces power consumption and demonstrates a prediction accuracy superior to benchmark schemes."

Source: Shibaura Institute of Technology

## Machine learning fine-tunes flash graphene

"Rice University scientists are using machine-learning techniques to streamline the process of synthesizing graphene from waste through flash Joule heating. The process discovered two years ago by the Rice lab of chemist James Tour has expanded beyond making graphene from various carbon sources to extracting other materials like metals from urban waste, with the promise of more environmentally friendly recycling to come.

The technique is the same for all of the above: blasting a jolt of high energy through the source material to eliminate all but the desired product. But the details for flashing each feedstock are different."

Source: Rice University

## Demystifying machine-learning systems

"Neural networks are sometimes called black boxes because, despite the fact that they can outperform humans on certain tasks, even the researchers who design them often don't understand how or why they work so well. But if a neural network is used outside the lab, perhaps to classify medical images that could help diagnose heart conditions, knowing how the model works helps researchers predict how it will behave in practice.

MIT researchers have now developed a method that sheds some light on the inner workings of black box neural networks. Modeled off the human brain, neural networks are arranged into layers of interconnected nodes, or "neurons," that process data. The new system can automatically produce descriptions of those

participants' impressions of their warmth, competence, social attractiveness, and hiring desirability. In Study 2, we examined how receiving assistance impacted interpersonal perceptions, and how perceptions might change whether the help was provided by AI or by another human. The results from both experiments suggest that the use of AI technologies can negatively influence perceptions of jobseekers."

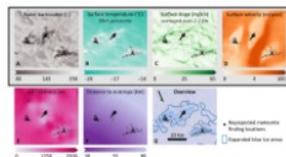
Source: Mary Ann Liebert

## The Impact of Artificial Intelligence on the Creativity of Videos

"This study explored the impact Artificial Intelligence (AI) has on the evaluation of creative elements in artistic videos. The aim was to verify to what extent the use of an AI algorithm (Style Transfer) contributes to changes in the perceived creativity of the videos. Creativity was evaluated in six quantitative items (Likert-type scale) and one qualitative question (qualitative description of the creativity expressed in the video by two words or expressions). Six videos were shown to both control (N = 49) and experimental group (N = 52) aiming at determining possible differences in creativity assessment criteria. Furthermore, both groups contained experts (Experimental, N = 27; Control, N = 25) and non-experts (Experimental, N = 25; Control, N = 24). The first round of videos composed of six videos that were the same for both the experimental and control condition (used to check for bias). No significant differences were found."

Source: ACM Digital Library

## MACHINE LEARNING



## Unexplored Antarctic meteorite collection sites revealed through machine learning

"Meteorites provide a unique view into the origin and evolution of the Solar System. Antarctica is the most productive region for recovering meteorites, where these extraterrestrial rocks concentrate at meteorite stranding zones. To date, meteorite-bearing blue ice areas are mostly identified by serendipity and through costly reconnaissance missions. Here, we identify meteorite-rich areas by combining state-of-the-art datasets in a machine learning algorithm and provide continent-wide estimates of the probability to find meteorites at any given location.

individual neurons, generated in English or another natural language."

Source: MIT

### **How well do explanation methods for machine-learning models work?**

"Imagine a team of physicians using a neural network to detect cancer in mammogram images. Even if this machine-learning model seems to be performing well, it might be focusing on image features that are accidentally correlated with tumors, like a watermark or timestamp, rather than actual signs of tumors.

To test these models, researchers use "feature-attribution methods," techniques that are supposed to tell them which parts of the image are the most important for the neural network's prediction. But what if the attribution method misses features that are important to the model? Since the researchers don't know which features are important to begin with, they have no way of knowing that their evaluation method isn't effective."

Source: MIT

### **Machine learning for morphable materials**

"Flat materials that can morph into three-dimensional shapes have potential applications in architecture, medicine, robotics, space travel, and much more. But programming these shape changes requires complex and time-consuming computations.

Now, researchers from the Harvard John A. Paulson School of Engineering and Applied Sciences (SEAS) have developed a platform that uses machine learning to program the transformation of 2D stretchable surfaces into specific 3D shapes.

"While machine learning methods have been classically employed for image recognition and language processing, they have also recently emerged as powerful tools to solve mechanics problems," said Katia Bertoldi, the William and Ami Kuan Danoff Professor of Applied Mechanics at SEAS and senior author of the study. "In this work we demonstrate that these tools can be extended to study the mechanics of transformable, inflatable systems."

Source: Harvard School of Engineering

### **Measuring trust in AI**

"Prompted by the increasing prominence of artificial intelligence (AI) in society, University of Tokyo researchers investigated public attitudes toward the ethics of AI. Their findings quantify how different demographics and ethical scenarios affect these attitudes. As part of this study, the team developed an octagonal visual metric, analogous to

The resulting set of ca. 600 meteorite stranding zones, with an estimated accuracy of over 80%, reveals the existence of unexplored zones, some of which are located close to research stations. Our analyses suggest that less than 15% of all meteorites at the surface of the Antarctic ice sheet have been recovered to date. The data-driven approach will greatly facilitate the quest to collect the remaining meteorites in a coordinated and cost-effective manner."

Source: Science Advances

### **(K)not machine learning**

"We review recent efforts to machine learn relations between knot invariants. Because these knot invariants have meaning in physics, we explore aspects of Chern-Simons theory and higher dimensional gauge theories. The goal of this work is to translate numerical experiments with Big Data to new analytic results."

Source: Cornell University

### **Driving style recognition using machine learning and smartphones**

"Background: The lack of real-time monitoring is one of the reasons for the lack of awareness among drivers of their dangerous driving behavior. This work aims to develop a driver profiling system where a smartphone's built-in sensors are used alongside machine learning algorithms to classify different driving behaviors.

Methods: We attempt to determine the optimal combination of smartphone sensors such as accelerometer, gyroscope, and GPS in order to develop an accurate machine learning algorithm capable of identifying different driving events (e.g. turning, accelerating, or braking).

Results: In our preliminary studies, we encountered some difficulties in obtaining consistent driving events, which had the potential to add "noise" to the observations, thus reducing the accuracy of the classification."

Source: F1000 Research

### **Machine learning reveals key ion selectivity mechanisms in polymeric membranes with subnanometer pores**

"Designing single-species selective membranes for high-precision separations requires a fundamental understanding of the molecular interactions governing solute transport. Here, we comprehensively assess molecular-level features that influence the separation of 18 different anions by nanoporous

a rating system, which could be useful to AI researchers who wish to know how their work may be perceived by the public.

Many people feel the rapid development of technology often outpaces that of the social structures that implicitly guide and regulate it, such as law or ethics. AI in particular exemplifies this as it has become so pervasive in everyday life for so many, seemingly overnight. This proliferation, coupled with the relative complexity of AI compared to more familiar technology, can breed fear and mistrust of this key component of modern living. Who distrusts AI and in what ways are matters that would be useful to know for developers and regulators of AI technology, but these kinds of questions are not easy to quantify."

Source: University of Tokyo

### Seeking a way of preventing audio models for AI machine learning from being fooled

"Researchers at the UPV/EHU-University of the Basque Country show that the distortion metrics used to detect intentional perturbations in audio signals are not a reliable measure of human perception, and have proposed a series of improvements. These perturbations, designed to be imperceptible, can be used to cause erroneous predictions in artificial intelligence. Distortion metrics are applied to assess how effective the methods are in generating such attacks."

Source: University of The Basque Country

### DEEP LEARNING



### Understanding human vision through Deep Learning

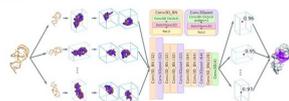
"This ERC-funded project is about the fundamental question of how our brain processes visual information," explains Tim Kietzmann, who is currently transitioning from the Donders Institute in the Netherlands to the Institute of Cognitive Science at Osnabrück University with his research group. "In vision, various processes naturally intertwine, rendering things complicated and exciting at the same time. With this project, we would like to take a closer look at this fascinating process: seeing involves information sampling via eye-movements and cortical filtering, information extraction, and information integration across space and time. All of these things happen in parallel within the fraction of a

cellulose acetate membranes. Our analysis identifies the limitations of bulk solvation characteristics to explain ion transport, highlighted by the poor correlation between hydration energy and the measured permselectivity ( $R^2 = 0.37$ ). Entropy-enthalpy compensation, spanning 40 kilojoules per mole, leads to a free-energy barrier ( $\Delta G^\ddagger$ ) variation of only ~8 kilojoules per mole across all anions. We apply machine learning to elucidate descriptors for energetic barriers from a set of 126 collected features. Notably, electrostatic features account for 75% of the overall features used to describe  $\Delta G^\ddagger$ , despite the relatively uncharged state of cellulose acetate. Our work presents an approach for studying ion transport across nanoporous membranes that could enable the design of ion-selective membranes."

Source: Science Advances

### DEEP LEARNING

Figure 1.



### Structure-based deep learning for binding site detection in nucleic acid macromolecules

"Structure-based drug design (SBDD) targeting nucleic acid macromolecules, particularly RNA, is a gaining momentum research direction that already resulted in several FDA-approved compounds. Similar to proteins, one of the critical components in SBDD for RNA is the correct identification of the binding sites for putative drug candidates. RNAs share a common structural organization that, together with the dynamic nature of these molecules, makes it challenging to recognize binding sites for small molecules. Moreover, there is a need for structure-based approaches, as sequence information only does not consider conformation plasticity of nucleic acid macromolecules. Deep learning holds a great promise to resolve binding site detection problem, but requires a large amount of structural data, which is very limited for nucleic acids, compared to proteins. In this study we composed a set of ~2000 nucleic acid-small molecule structures comprising ~2500 binding sites, which is ~40-times larger than previously used one, and demonstrated the first structure-based deep learning approach, BiteNetN, to detect binding sites in nucleic acid structures."

Source: Oxford Academic

### Biometrics-protected optical communication enabled by

second across a large variety of brain areas. That is, the brain not only deciphers what it is that it is seeing, but at the same time decides when and where to look next to gather further information. To better understand these interrelated processes, we will combine high-resolution measurements of brain waves during natural vision, and analyze these data using machine learning techniques and simulate them in large-scale computational models. The cognitive science department at Osnabrück is the ideal place for this research!"

Source: Osnabrück University

### **New project to improve performance of deep learning models**

"A graph is a structured way to represent data, with nodes representing entities and edges representing the relationships between these entities. GNNs provide an easy way to conduct node-level, edge-level, and graph-level prediction via machine learning. However, they usually require a large amount of label information to train the model parameters. According to He, the lack of labeled data in graphs can render many existing deep learning models ineffective in achieving the desired performance. Her new project involves a work-around so that GNNs can use unlabeled data and other relevant information.

"For example, in fraud detection, the number of known fraudulent transactions is usually very small compared to the total number of transactions, hence the lack of labeled data. Most existing GNN models tend to suffer from such label scarcity. In my new project, we aim to address this issue by leveraging weak supervision or additional information (besides the limited label information), such as labeled data from other related applications and/or access to a domain expert, in order to compensate for the lack of labeled data," said He."

Source: University of Illinois School of Information Sciences

### **deep learning-enhanced triboelectric/photonic synergistic interface**

"Security is a prevailing concern in communication as conventional encryption methods are challenged by progressively powerful supercomputers. Here, we show that biometrics-protected optical communication can be constructed by synergizing triboelectric and nanophotonic technology. The synergy enables the loading of biometric information into the optical domain and the multiplexing of digital and biometric information at zero power consumption. The multiplexing process seals digital signals with a biometric envelope to avoid disrupting the original high-speed digital information and enhance the complexity of transmitted information. The system can perform demultiplexing, recover high-speed digital information, and implement deep learning to identify 15 users with around 95% accuracy, irrespective of biometric information data types (electrical, optical, or demultiplexed optical)."

Source: Science Advances

### **Inverse design of soft materials via a deep learning-based evolutionary strategy**

"Colloidal self-assembly—the spontaneous organization of colloids into ordered structures—has been considered key to produce next-generation materials. However, the present-day staggering variety of colloidal building blocks and the limitless number of thermodynamic conditions make a systematic exploration intractable. The true challenge in this field is to turn this logic around and to develop a robust, versatile algorithm to inverse design colloids that self-assemble into a target structure. Here, we introduce a generic inverse design method to efficiently reverse-engineer crystals, quasicrystals, and liquid crystals by targeting their diffraction patterns. Our algorithm relies on the synergetic use of an evolutionary strategy for parameter optimization, and a convolutional neural network as an order parameter, and provides a way forward for the inverse design of experimentally feasible colloidal interactions, specifically optimized to stabilize the desired structure."

Source: Science Advances

### **High-throughput screening platform for quantitative phenotype analysis of *Xenopus laevis* with deep learning**

"*Xenopus laevis* are emerging models to study human diseases and to

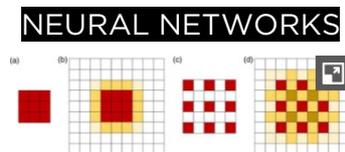
investigate pharmaceutical effects in vivo due to smaller size and faster developmental rates. It is also an effective organism to observe drug effects on phenotypic characteristics because it can provide many biological systems in a short time and remain optically accessible at the early stages of development. Although morphological evaluation of massive *Xenopus* data is an essential procedure, it requires labor-intensive and manual inspection under an optical microscope. In this study, we propose a high-throughput, widefield, and time-lapse phenotype screening system modifying the office scanner. We also fabricated the customized PDMS well plate for efficient and stress-free imaging of living *Xenopus laevis* samples in normal and drug environments.”

Source: SPIE

### **DeepKE: A Deep Learning Based Knowledge Extraction Toolkit for Knowledge Base Population**

“We present a new open-source and extensible knowledge extraction toolkit, called DeepKE (Deep learning based Knowledge Extraction), supporting standard fully supervised, low-resource few-shot and document-level scenarios. DeepKE implements various information extraction tasks, including named entity recognition, relation extraction and attribute extraction. With a unified framework, DeepKE allows developers and researchers to customize datasets and models to extract information from unstructured texts according to their requirements. Specifically, DeepKE not only provides various functional modules and model implementation for different tasks and scenarios but also organizes all components by consistent frameworks to maintain sufficient modularity and extensibility.”

Source: Cornell University



### **Obstacle type recognition in visual images via dilated convolutional neural network for unmanned surface vehicles**

“Recognition of obstacle type based on visual sensors is important for navigation by unmanned surface vehicles (USV), including path planning, obstacle avoidance, and reactive control. Conventional detection techniques may fail to distinguish obstacles that are similar in visual appearance in a cluttered environment. This work proposes a

novel obstacle type recognition approach that combines a dilated operator with the deep-level features map of ResNet50 for autonomous navigation. First, visual images are collected and annotated from various different scenarios for USV test navigation. Second, the deep learning model, based on a dilated convolutional neural network, is set and trained."

Source: Cambridge University Press

### **Individual Treatment Effect Estimation Through Controlled Neural Network Training in Two Stages**

"We develop a Causal-Deep Neural Network (CDNN) model trained in two stages to infer causal impact estimates at an individual unit level. Using only the pre-treatment features in stage 1 in the absence of any treatment information, we learn an encoding for the covariates that best represents the outcome. In the 2nd stage we further seek to predict the unexplained outcome from stage 1, by introducing the treatment indicator variables alongside the encoded covariates. We prove that even without explicitly computing the treatment residual, our method still satisfies the desirable local Neyman orthogonality, making it robust to small perturbations in the nuisance parameters. Furthermore, by establishing connections with the representation learning approaches, we create a framework from which multiple variants of our algorithm can be derived. We perform initial experiments on the publicly available data sets to compare these variants and get guidance in selecting the best variant of our CDNN method."

Source: Cornell University

### **Three-dimensional finite-time guidance law based on sliding mode adaptive RBF neural network against a highly manoeuvring target**

"In order to intercept a highly manoeuvring target with an ideal impact angle in the three-dimensional space, this paper promises to probe into the problem of three-dimensional terminal guidance. With the goal of the highly target acceleration and short terminal guidance time, a guidance law, based on the advanced fast non-singular terminal sliding mode theory, is designed to quickly converge the line-of-sight (LOS) angle and the LOS angular rate within a finite time. In the design process, the target acceleration is regarded as an unknown boundary external disturbance of the guidance system, and the RBF neural network is used to

estimate it. In order to improve the estimation accuracy of RBF neural network and accelerate its convergence, the parameters of RBF neural network are adjusted online in real time."

Source: Cambridge University Press

### **Bolt preload monitoring based on percussion sound signal and convolutional neural network**

"The general approach to percussion-based monitoring of bolt preload is to train a classifier model to map the preloads and acoustic characteristics of percussion signals. However, the traditional percussion-based approach can only classify the preloads of bolts into certain ranges, and cannot accurately predict the exact bolt preload. This paper proposes an approach to estimate bolt preload using a convolutional neural network (CNN). The frequency contents of the percussion signals are analysed with the Fast Fourier Transform (FFT), and the magnitudes of signals in different frequencies ranges are reconstructed into a matrix, which can be treated as an image. Each image is labelled with the corresponding bolt preload. Then the labelled images are used to train the CNN model, and the trained model is used to detect the actual preload of a selected bolt."

Source: Taylor & Francis Online

### **Fusing Convolutional Neural Network and Geometric Constraint for Image-Based Indoor Localization**

"This letter proposes a new image-based localization framework that explicitly localizes the camera/robot by fusing Convolutional Neural Network (CNN) and sequential images' geometric constraints. The camera is localized using a single or few observed images and training images with 6-degree-of-freedom pose labels. A Siamese network structure is adopted to train an image descriptor network, and the visually similar candidate image in the training set is retrieved to localize the testing image geometrically. Meanwhile, a probabilistic motion model predicts the pose based on a constant velocity assumption. The two estimated poses are finally fused using their uncertainties to yield an accurate pose prediction. This method leverages the geometric uncertainty and is applicable in indoor scenarios predominated by diffuse illumination. Experiments on simulation and real data sets demonstrate the efficiency of our proposed method."

Source: IEEE Xplore

## OPERATIONS MANAGEMENT



### **Preface: artificial intelligence in operations management**

"The recent and exponential growth of adopters of digital technologies, thanks to the information and communications technologies (ICTs) advances, have been changing the field of operations management (OM) drastically (Li, 2020; Queiroz & Fosso Wamba, 2021). In this perspective, although artificial intelligence (AI) has already been discussed for decades (Fosso Wamba et al., 2021), only in recent years, supported by the unprecedented advances in computer processing power, internet diffusion, and social networks sites, it has gained popularization as never before seen. In this outlook, the organizations started a run to mindset shift to incorporate AI techniques into their operations (Belhadi et al., 2021). Thus, it can be seen that AI has been used successfully in many operations contexts (Fosso Wamba & Queiroz, 2021; Queiroz & Fosso Wamba, 2021; Yang et al., 2021)."

Source: Springer Link

### **Design and interactive performance of human resource management system based on artificial intelligence**

"The purpose is to strengthen Human Resources Management (HRM) through information management using Artificial Intelligence (AI) technology. First, the selection criteria of the applicant's resume during recruitment and the formulation standards of the contract salary are analyzed. Then, the resume information is extracted and converted into the data-type format. Besides, the salary forecast model in the HRM system (HRMS) is designed based on the Back Propagation Neural Network (BPNN), and network structure, parameter initialization, and activation function of the BPNN are selected and optimized. The experimental results demonstrate that the algorithm optimized by the Nadm has shown improved convergence speed and forecast effect, with 187 iterations."

Source: PLOS One

## HEALTHCARE

Fig. 1: Flow diagram of screening strategy.



## Guidelines and quality criteria for artificial intelligence-based prediction models in healthcare: a scoping review

“While the opportunities of ML and AI in healthcare are promising, the growth of complex data-driven prediction models requires careful quality and applicability assessment before they are applied and disseminated in daily practice. This scoping review aimed to identify actionable guidance for those closely involved in AI-based prediction model (AIPM) development, evaluation and implementation including software engineers, data scientists, and healthcare professionals and to identify potential gaps in this guidance. We performed a scoping review of the relevant literature providing guidance or quality criteria regarding the development, evaluation, and implementation of AIPMs using a comprehensive multi-stage screening strategy. PubMed, Web of Science, and the ACM Digital Library were searched, and AI experts were consulted.”

Source: Nature

## Biomedical Applications of Computer Vision using Artificial Intelligence

“Computational neuroscience is concerned with simulating real neural systems to predict brain workings and disorders from subneuronal systems to network plasticity as hypotheses to be tested later in real neural tissues and hence to understand the principles governing them. Some ideas from this field can be used in artificial intelligence and other fields. Mimicking the central nervous system and by extension and creating various additional methods of computation such as artificial neural networks, machine learning, deep learning, or genetic algorithms have led to the artificial intelligence field which aims to solve given problems in a flexible, intelligent, and learnable way. The advent of these fields has numerous biomedical applications such as image processing and computer vision, machine learning, and deep learning for the assessment of imaging and signal datasets, disease diagnostic systems, expert systems to offer and optimize treatment planning, brain-computer

interface, smart prosthetic limbs, and  
many others."  
Source: Hindawi

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