Machine Learning Design Proteins

According to researchers at Massachusetts Institute of Technology (MIT) in the US they both gain from being composed of structures over a range of scales be that notes, chords and melodies or amino acids, proteins and collagen matrices. [29]

"We basically combined advances in neural networks and machine-learning with quantum Monte Carlo tools," says Savona, referring to a large toolkit of computational methods that physicists use to study complex quantum systems. [28]

As cosmologists and astrophysicists delve deeper into the darkest recesses of the universe, their need for increasingly powerful observational and computational tools has expanded exponentially. [27]

Now, a team of scientists at MIT and elsewhere has developed a neural network, a form of artificial intelligence (AI), that can do much the same thing, at least to a limited extent: It can read scientific papersand render a plain-English summary in a sentence or two. [26]

To address this gap in the existing literature, a team of researchers at SRI International has created a human-AI image guessing game inspired by the popular game 20 Questions (20Q), which can be used to evaluate the helpfulness of machine explanations. [25]

Social, economic, environmental and health inequalities within cities can be detected using street imagery. [24]

Citizen science is a boon for researchers, providing reams of data about everything from animal species to distant galaxies. [23]

In early 2018, with support from IBM Corporate Citizenship and the Danish Ministry for Foreign Affairs, IBM and the Danish Refugee Council (DRC) embarked on a partnership aimed squarely at the need to better understand migration drivers and evidence-based policy guidance for a range of stakeholders. [22]

Scientists at the Allen Institute have used machine learning to train computers to see parts of the cell the human eye cannot easily distinguish. [21]

Small angle X-ray scattering (SAXS) is one of a number of biophysical techniques used for determining the structural characteristics of biomolecules. [20]

A deep neural network running on an ordinary desktop computer is interpreting highly technical data related to national security as well as—and sometimes better than— today's best automated methods or even human experts. [19]

Scientists at the National Center for Supercomputing Applications (NCSA), located at the University of Illinois at Urbana-Champaign, have pioneered the use of GPU-accelerated deep learning for rapid detection and characterization of gravitational waves. [18]

Researchers from Queen Mary University of London have developed a mathematical model for the emergence of innovations. [17]

Quantum computers can be made to utilize effects such as quantum coherence and entanglement to accelerate machine learning. [16]

Neural networks learn how to carry out certain tasks by analyzing large amounts of data displayed to them. [15]

Who is the better experimentalist, a human or a robot? When it comes to exploring synthetic and crystallization conditions for inorganic gigantic molecules, actively learning machines are clearly ahead, as demonstrated by British Scientists in an experiment with polyoxometalates published in the journal Angewandte Chemie. [14]

Machine learning algorithms are designed to improve as they encounter more data, making them a versatile technology for understanding large sets of photos such as those accessible from Google Images. Elizabeth Holm, professor of materials science and engineering at Carnegie Mellon University, is leveraging this technology to better understand the enormous number of research images accumulated in the field of materials science. [13]

With the help of artificial intelligence, chemists from the University of Basel in Switzerland have computed the characteristics of about two million crystals made up of four chemical elements. The researchers were able to identify 90 previously unknown thermodynamically stable crystals that can be regarded as new materials. [12]

The artificial intelligence system's ability to set itself up quickly every morning and compensate for any overnight fluctuations would make this fragile technology much more useful for field measurements, said co-lead researcher Dr Michael Hush from UNSW ADFA. [11]

Quantum physicist Mario Krenn and his colleagues in the group of Anton Zeilinger from the Faculty of Physics at the University of Vienna and the Austrian Academy of Sciences have developed an algorithm which designs new useful quantum experiments. As the computer does not rely on human intuition, it finds novel unfamiliar solutions. [10]

Researchers at the University of Chicago's Institute for Molecular Engineering and the University of Konstanz have demonstrated the ability to generate a quantum logic operation, or rotation of the qubit, that - surprisingly—is intrinsically resilient to noise as well as to variations in the strength or duration of the control. Their achievement is

based on a geometric concept known as the Berry phase and is implemented through entirely optical means within a single electronic spin in diamond. [9]

New research demonstrates that particles at the quantum level can in fact be seen as behaving something like billiard balls rolling along a table, and not merely as the probabilistic smears that the standard interpretation of quantum mechanics suggests. But there's a catch - the tracks the particles follow do not always behave as one would expect from "realistic" trajectories, but often in a fashion that has been termed "surrealistic." [8]

Quantum entanglement—which occurs when two or more particles are correlated in such a way that they can influence each other even across large distances—is not an all-or-nothing phenomenon, but occurs in various degrees. The more a quantum state is entangled with its partner, the better the states will perform in quantum information applications. Unfortunately, quantifying entanglement is a difficult process involving complex optimization problems that give even physicists headaches. [7]

A trio of physicists in Europe has come up with an idea that they believe would allow a person to actually witness entanglement. Valentina Caprara Vivoli, with the University of Geneva, Pavel Sekatski, with the University of Innsbruck and Nicolas Sangouard, with the University of Basel, have together written a paper describing a scenario where a human subject would be able to witness an instance of entanglement—they have uploaded it to the arXiv server for review by others. [6]

The accelerating electrons explain not only the Maxwell Equations and the Special Relativity, but the Heisenberg Uncertainty Relation, the Wave-Particle Duality and the electron's spin also, building the Bridge between the Classical and Quantum Theories.

The Planck Distribution Law of the electromagnetic oscillators explains the electron/proton mass rate and the Weak and Strong Interactions by the diffraction patterns. The Weak Interaction changes the diffraction patterns by moving the electric charge from one side to the other side of the diffraction pattern, which violates the CP and Time reversal symmetry.

The diffraction patterns and the locality of the self-maintaining electromagnetic potential explains also the Quantum Entanglement, giving it as a natural part of the relativistic quantum theory.

Contents

Preface

Physicists are continually looking for ways to unify the theory of relativity, which describes largescale phenomena, with quantum theory, which describes small-scale phenomena. In a new proposed experiment in this area, two toaster-sized "nanosatellites" carrying entangled condensates orbit around the Earth, until one of them moves to a different orbit with different gravitational field strength. As a result of the change in gravity, the entanglement between the condensates is predicted to degrade by up to 20%. Experimentally testing the proposal may be possible in the near future. [5]

Quantum entanglement is a physical phenomenon that occurs when pairs or groups of particles are generated or interact in ways such that the quantum state of each particle cannot be described independently – instead, a quantum state may be given for the system as a whole. [4]

I think that we have a simple bridge between the classical and quantum mechanics by understanding the Heisenberg Uncertainty Relations. It makes clear that the particles are not point like but have a dx and dp uncertainty.

Amino acid orchestra trains machine learning algorithms to design proteins

Ever wondered what Beethoven and bone have in common? According to researchers at Massachusetts Institute of Technology (MIT) in the US they both gain from being composed of structures over a range of scales be that notes, chords and melodies or amino acids, proteins and collagen matrices. Taking the analogy further Markus Buehler and colleagues have translated the vibrations of amino acids and the longer-range structures of the proteins they form into a musical framework. Machine learning algorithms trained on this musically transcribed protein data could devise fresh amino acid music based on musical principals learnt from the training data set, which the researchers then translate back into protein structures.

 "What we've been trying to do in a lot of different ways is to find ways of predicting a protein's functionality from its sequence and that's a really difficult thing to do," Buehler tells *Physics World*. For several years Markus Buehler and his group at MIT have studied materials including spiders' webs and nacre to identify the hierarchical structures behind their impressive mechanical properties. He explains that current approaches to relating protein structure and function generally rely on long computational-resource-hungry molecular dynamics simulations to solve equations approximating the quantum mechanical interactions at the molecular scale in order to determine how the protein folds, and how it functions. "One of the directions we have pursued is to think how we look at materials, and we realized that when we look at materials at the molecular scale, the atoms and molecules continuously vibrate. So we thought that maybe there's a way of capturing the spectrum of vibrations at the nanoscale and building a model from that."

Based on the vibrational frequencies of amino acids the researchers developed an amino acid musical scale. They then encoded secondary structures that govern the way the proteins fold into other musical components such as rhythm and volume. Just as pictorial representations of data can make it easier to recognize patterns and trends, presenting the algorithm with a musical representation of the data may help identify relationships that have so far remained elusive, and already the results are promising.

Markus Buehler, Professor in Engineering at Massachusetts Institute of Technology (MIT) in the US. Credit: MIT

"Based on a training [data] set, we can now come up with proteins that nature has not invented before," says Buehler. "We've also found that some of the proteins that our AI method can generate are proteins that nature has invented, but they were not part of the training sets – it's really fascinating that the method can sort of discover things that evolution has already discovered on its own. And this leads to the application of this work, that we're now able to optimize protein sequences using this method because we can ask the AI to generate a large number of candidates, which we can then further categorize."

Musical inspiration

Training a machine learning algorithm on an amino acid orchestra to discover new useful materials may seem a neat if unorthodox idea, but successfully putting it into practice has built on over a decade of work exploring the function and properties of hierarchical structures and the translation of theoretical models into different frameworks. As well as this unique catalogue of expertise in Buehler's group, developments in AI have been crucial to making use of the approach.

Unlike classical western music, where each scale is made up of 12 notes separated by semitones, the amino acid scale has 20 tones, and sounds very different. Using the musical representation of proteins to reveal insights into the relationships between protein structures at different levels and their functions, requires not just a familiarization with this strange sounding music but the ability to ignore the principals of classical music.

"AI was a way of overcoming that limitation, to have a neutral model that has never heard any music but basically learned only from the data that was provided," says Buehler. "Because one of the problems you have with a human brain, is that if you want to compose a new protein you tend to want to make it sound like the music you've heard before – this is sort of how composition works we're trying to create or explore ideas, themes, chord progressions and so on that you have maybe heard before. Of course, in this case it doesn't work, because these core progressions and melodies and successions of notes, might not at all relate to anything that's important for protein." While the system has already identified real and potentially realisable proteins, future work will require improved data sets to train the algorithms with the aim of identifying protein structures with specific folding and functional properties.

Unifying trends

Buehler is also optimistic about other sectors that could benefit from a musical representation of data. "Generally, I think there's a very interesting fundamental insight that one can possibly get from this kind of work. An extension of this work would be the idea that many of these hierarchical systems actually show striking similarities in the way they're built." He describes the way materials like spider silk, bone, and nacre, or language or music share similarities in the way they are constructed to give rise to various functions from simple building blocks. "One of the general things I think that we could explore is whether we have discovered certain features or ways systems can be designed better in other representations."

You can hear compositions from these musical representations on soundcloud or download an app to play with them yourself. Full details of the work applied to protein research are reported in *ACS Nano*. [29]

Simulating quantum systems with neural networks

Even on the scale of everyday life, nature is governed by the laws of quantum physics. These laws explain common phenomena like light, sound, heat, or even the trajectories of balls on a pool table. But when applied to a large number of interacting particles, the laws of quantum physics actually predict a variety of phenomena that defy intuition.

In order to study quantum systems made of many particles, physicists must first be able to simulate them. This can be done by solving the equations describing their inner workings on supercomputers. But while Moore's Law predicts that the processing power of computers doubles every couple of years, this is a far cry from the power needed to tackle the challenges of quantum physics.

The reason is that predicting the properties of a quantum system is enormously complex, demanding a computational power that grows exponentially with the size of the quantum system—an "intrinsically complex" task, according to Professor Vincenzo Savona, who directs the Laboratory of Theoretical Physics of Nanosystems at EPFL.

"Things become even more complicated when the quantum system is open, meaning that it is subject to the disturbances of its surrounding environment," Savona adds. And yet, tools to efficiently simulate open quantum systems are much needed, as most modern experimental platforms for quantum science and technology are open systems, and physicists are constantly in search of new ways to simulate and benchmark them.

But significant progress has been made thanks to a new computational method that simulates quantum systems with neural networks. The method was developed by Savona and his Ph.D. student Alexandra Nagy at EPFL—and independently by scientists at Université Paris Diderot, the Heriot-Watt University in Edinburgh, and the Flatiron Institute in New York. The total body of work is being published across three papers in *Physical Review Letters*.

"We basically combined advances in neural networks and machine-learning with quantum Monte Carlo tools," says Savona, referring to a large toolkit of computational methods that physicists use to study complex quantum systems. The scientists trained a neural network to represent simultaneously the many quantum states in which a quantum system can be cast by the influence of its environment.

The neural-network approach allowed the physicists to predict the properties of quantum systems of considerable size and arbitrary geometry. "This is a novel computational approach that addresses the problem of open quantum systems with versatility and a lot of potential for scaling up," says Savona. The method is set to become a tool of choice for the study of complex quantum systems, and, looking a bit more into the future, for assessing the effects of noise on quantum hardware. [28]

CosmoGAN: Training a neural network to study dark matter

As cosmologists and astrophysicists delve deeper into the darkest recesses of the universe, their need for increasingly powerful observational and computational tools has expanded exponentially. From facilities such as the Dark Energy Spectroscopic Instrument to supercomputers like Lawrence Berkeley National Laboratory's Cori system at the National Energy Research Scientific Computing (NERSC) facility, they are on a quest to collect, simulate, and analyze increasing amounts of data that can help explain the nature of things we can't see, as well as those we can.

Toward this end, gravitational lensing is one of the most promising tools scientists have to extract this information by giving them the ability to probe both the geometry of the universe and the growth of cosmic structure. Gravitational lensing distorts images of distant galaxies in a way that is determined by the amount of matter in the line of sight in a certain direction, and it provides a way of looking at a two-dimensional map of dark matter, according to Deborah Bard, Group Lead for the Data Science Engagement Group in Berkeley Lab's National Energy Research Scientific Computing Center (NERSC).

"Gravitational lensing is one of the best ways we have to study dark matter, which is important because it tells us a lot about the structure of the universe," she said. "The majority of matter in the universe is dark matter, which we can't see directly, so we have to use indirect methods to study how it is distributed."

But as experimental and theoretical datasets grow, along with the simulations needed to image and analyze this data, a new challenge has emerged: these simulations are increasingly—even prohibitively—computationally expensive. So computational cosmologists often resort to computationally cheaper surrogate models, which emulate expensive simulations. More recently, however, "advances in deep generative models based on neural networks opened the possibility of constructing more robust and less hand-engineered surrogate models for many types of simulators, including those in cosmology," said Mustafa Mustafa, a machine learning engineer at NERSC and lead author on a new study that describes one such approach developed by a collaboration involving Berkeley Lab, Google Research, and the University of KwaZulu-Natal.

A variety of deep generative models are being investigated for science applications, but the Berkeley Lab-led team is taking a unique tack: generative adversarial networks (GANs). In a paper published May 6, 2019 in *Computational Astrophysics and Cosmology*, they discuss their new deep learning network, dubbed CosmoGAN, and its ability to create high-fidelity, weak gravitational lensing convergence maps.

"A convergence map is effectively a 2-D map of the gravitational lensing that we see in the sky along the line of sight," said Bard, a co-author on the *Computational Astrophysics and Cosmology* paper. "If you have a peak in a convergence map that corresponds to a peak in a large amount of matter along the line of sight, that means there is a huge amount of dark matter in that direction."

The Advantages of GANs

Why opt for GANs instead of other types of generative models? Performance and precision, according to Mustafa.

"From a deep learning perspective, there are other ways to learn how to generate convergence maps from images, but when we started this project GANs seemed to produce very high-resolution images compared to competing methods, while still being computationally and neural network size efficient," he said.

"We were looking for two things: to be accurate and to be fast," added co-author Zaria Lukic, a research scientist in the Computational Cosmology Center at Berkeley Lab. "GANs offer hope of being nearly as accurate compared to full physics simulations."

The research team is particularly interested in constructing a surrogate model that would reduce the computational cost of running these simulations. In the *Computational Astrophysics and Cosmology* paper, they outline a number of advantages of GANs in the study of large physics simulations.

"GANs are known to be very unstable during training, especially when you reach the very end of the training and the images start to look nice—that's when the updates to the network can be really chaotic," Mustafa said. "But because we have the summary statistics that we use in cosmology, we were able to evaluate the GANs at every step of the training, which helped us determine the generator we thought was the best. This procedure is not usually used in training GANs."

Using the CosmoGAN generator network, the team has been able to produce convergence maps that are described by—with high statistical confidence—the same summary statistics as the fully simulated maps. This very high level of agreement between convergence maps that are statistically indistinguishable from maps produced by physics-based generative models offers an important step toward building emulators out of deep neural networks.

"The huge advantage here was that the problem we were tackling was a physics problem that had associated metrics," Bard said. "But with our approach, there are actual metrics that allow you to quantify how accurate your GAN is. To me that is what is really exciting about this—how these kinds of physics problems can influence machine learning methods.

Ultimately such approaches could transform science that currently relies on detailed physics simulations that require billions of compute hours and occupy petabytes of disk space—but there is considerable work still to be done. Cosmology data (and scientific data in general) can require very high-resolution measurements, such as full-sky telescope images.

"The 2-D images considered for this project are valuable, but the actual physics simulations are 3-D and can be time-varying ?and irregular, producing a rich, web-like structure of features," said Wahid Bhmiji, a big data architect in the Data and Analytics Services group at NERSC and a co-author on the *Computational Astrophysics and Cosmology* paper. "In addition, the approach needs to be extended to explore new virtual universes rather than ones that have already been simulated—ultimately building a controllable CosmoGAN."

"The idea of doing controllable GANs is essentially the Holy Grail of the whole problem that we are working on: to be able to truly emulate the physical simulators we need to build surrogate models based on controllable GANs," Mustafa added. "Right now we are trying to understand how to stabilize the training dynamics, given all the advances in the field that have happened in the last couple of years. Stabilizing the training is extremely important to actually be able to do what we want to do next." [27]

A neural network can read scientific papers and render a plain-English summary

The work of a science writer, including this one, includes reading journal papers filled with specialized technical terminology, and figuring out how to explain their contents in language that readers without a scientific background can understand.

Now, a team of scientists at MIT and elsewhere has developed a neural network, a form of artificial intelligence (AI), that can do much the same thing, at least to a limited extent: It can read scientific papers and render a plain-English summary in a sentence or two.

Even in this limited form, such a neural network could be useful for helping editors, writers, and scientists scan a large number of papers to get a preliminary sense of what they're about. But the approach the team developed could also find applications in a variety of other areas besides language processing, including machine translation and speech recognition.

The work is described in the journal *Transactions of the Association for Computational Linguistics*, in a paper by Rumen Dangovski and Li Jing, both MIT graduate students; Marin Soljačić, a professor of physics at MIT; Preslav Nakov, a senior scientist at the Qatar Computing Research Institute, HBKU; and Mićo Tatalović, a former Knight Science Journalism fellow at MIT and a former editor at *New Scientist* magazine.

From AI for physics to natural language

The work came about as a result of an unrelated project, which involved developing new artificial intelligence approaches based on neural networks, aimed at tackling certain thorny problems in physics. However, the researchers soon realized that the same approach could be used to address other difficult computational problems, including natural language processing, in ways that might outperform existing neural network systems.

"We have been doing various kinds of work in AI for a few years now," Soljačić says. "We use AI to help with our research, basically to do physics better. And as we got to be more familiar with AI, we would notice that every once in a while there is an opportunity to add to the field of AI because of something that we know from physics—a certain mathematical construct or a certain law in physics. We noticed that hey, if we use that, it could actually help with this or that particular AI algorithm."

This approach could be useful in a variety of specific kinds of tasks, he says, but not all. "We can't say this is useful for all of AI, but there are instances where we can use an insight from physics to improve on a given AI algorithm."

Neural networks in general are an attempt to mimic the way humans learn certain new things: The computer examines many different examples and "learns" what the key underlying patterns are. Such systems are widely used for pattern recognition, such as learning to identify objects depicted in photos.

But neural networks in general have difficulty correlating information from a long string of data, such as is required in interpreting a research paper. Various tricks have been used to improve this capability, including techniques known as long short-term memory (LSTM) and gated recurrent

units (GRU), but these still fall well short of what's needed for real natural-language processing, the researchers say.

The team came up with an alternative system, which instead of being based on the multiplication of matrices, as most conventional neural networks are, is based on vectors rotating in a multidimensional space. The key concept is something they call a rotational unit of memory (RUM).

Essentially, the system represents each word in the text by a vector in multidimensional space—a line of a certain length pointing in a particular direction. Each subsequent word swings this vector in some direction, represented in a theoretical space that can ultimately have thousands of dimensions. At the end of the process, the final vector or set of vectors is translated back into its corresponding string of words.

"RUM helps neural networks to do two things very well," Nakov says. "It helps them to remember better, and it enables them to recall information more accurately."

After developing the RUM system to help with certain tough physics problems such as the behavior of light in complex engineered materials, "we realized one of the places where we thought this approach could be useful would be natural language processing," says Soljačić, recalling a conversation with Tatalović, who noted that such a tool would be useful for his work as an editor trying to decide which papers to write about. Tatalović was at the time exploring AI in science journalism as his Knight fellowship project.

"And so we tried a few natural language processing tasks on it," Soljačić says. "One that we tried was summarizing articles, and that seems to be working quite well."

The proof is in the reading

As an example, they fed the same research paper through a conventional LSTM-based neural network and through their RUM-based system. The resulting summaries were dramatically different.

The LSTM system yielded this highly repetitive and fairly technical summary: "Baylisascariasis," kills mice, has endangered the allegheny woodrat and has caused disease like blindness or severe consequences. This infection, termed "baylisascariasis," kills mice, has endangered the allegheny woodrat and has caused disease like blindness or severe consequences. This infection, termed "baylisascariasis," kills mice, has endangered the allegheny woodrat.

Based on the same paper, the RUM system produced a much more readable summary, and one that did not include the needless repetition of phrases: Urban raccoons may infect people more than previously assumed. 7 percent of surveyed individuals tested positive for raccoon roundworm antibodies. Over 90 percent of raccoons in Santa Barbara play host to this parasite.

Already, the RUM-based system has been expanded so it can "read" through entire research papers, not just the abstracts, to produce a summary of their contents. The researchers have even tried using the system on their own research paper describing these findings—the paper that this news story is attempting to summarize.

Here is the new neural network's summary: Researchers have developed a new representation process on the rotational unit of RUM, a recurrent memory that can be used to solve a broad spectrum of the neural revolution in natural language processing.

It may not be elegant prose, but it does at least hit the key points of information.

Çağlar Gülçehre, a research scientist at the British AI company Deepmind Technologies, who was not involved in this work, says this research tackles an important problem in neural networks, having to do with relating pieces of information that are widely separated in time or space. "This problem has been a very fundamental issue in AI due to the necessity to do reasoning over long time-delays in sequence-prediction tasks," he says. "Although I do not think this paper completely solves this problem, it shows promising results on the long-term dependency tasks such as question-answering, text summarization, and associative recall."

Gülçehre adds, "Since the experiments conducted and model proposed in this paper are released as open-source on Github, as a result many researchers will be interested in trying it on their own tasks. … To be more specific, potentially the approach proposed in this paper can have very high impact on the fields of natural language processing and reinforcement learning, where the long-term dependencies are very crucial." [26]

ExAG: An image-guessing game to evaluate the helpfulness of machine explanations

In recent years, researchers have been trying to make artificial intelligence (AI) more transparent by developing algorithms that can explain their actions and behavior, as this could encourage greater trust in machines and enhance human-AI interactions. Despite their efforts, so far very few studies have tangibly evaluated the impact of AI explanations on the performance achieved in tasks that involve human-AI collaboration.

To address this gap in the existing literature, a team of researchers at SRI International has created a human-AI image guessing game inspired by the popular game 20 Questions (20Q), which can be used to evaluate the helpfulness of machine explanations. Their paper, recently published on arXiv, is among the first to explore the effects of developing more 'explainable' AI.

"The idea came about while we were working on a DARPA project," Arijit Ray, a computer scientist at SRI International who carried out the study, told TechXolore. "In this project, we are developing explainable AI systems, which not only generate the desired output (e.g. object detection, answers to questions, etc.) but also explanations of how they arrived at that output. We needed a mechanism to evaluate whether the additional explanations provided by AIs were useful for the user to gain a better understanding of the AI systems. To this end, we created an interactive human-AI collaborative task, Explanation-assisted GuessWhich (ExAG), which is an adaptation of the famous 20Q game, to demonstrate the effectiveness of the various machine explanation techniques that we are developing."

The image-guessing game developed by Ray and his colleagues closely resembles the popular game 20 Questions, which usually involves two players. In 20Q, one player thinks about something and the second player tries to guess what it is by asking 20 closed-ended questions (i.e., questions that can only be answered with 'yes' or 'no').

In ExAG, the adaptation of the game devised by Ray and his colleagues, a user is shown five images, one of which has been chosen by the AI system as the 'secret image.' Essentially, the user needs to figure out which one among the pictures he/she saw is the 'secret image,' by asking natural language questions about it.

In contrast with the traditional 20Q game, in ExAG human users can ask both closed and open-ended questions. For instance, they could ask 'what is in the image?,' 'where was the image taken?' and so on. The AI system answers a user's questions one at a time and can optionally explain its answers.

Based on these answers, the user will then try to guess the image that the AI had originally selected. The overall goal of the game is to correctly identify the 'secret image' by asking as few questions as possible.

"The AI system provides two modes of explanations, visual and textual," Ray explained. "For visual explanations, the AI system generates heat maps highlighting the regions that support its answers. For example, if a user asks what is in the image, and it looks like a dog, the AI will highlight the dog region and say this is what leads to the answer 'it's a dog.' For textual explanations, on the other hand, the AI system provides answers to related questions for each of the images. So, if you ask what a person is doing and the answer is surfing, for instance, it will also answer related questions like 'what do I see in the image? A surfer.' 'Where is the picture taken? A beach.'

Due to the nature of the image-guessing game, the quality of the answers and explanations provided by the AI can significantly affect a human user's success and performance. It is worth noting that current state-of-the-art performance in visual question answering is around 65 percent, which means that the AI system generates correct answers 65 percent of the time.

Ray and his colleagues observed that users typically succeeded in ExAG by taking advantage of the AIs explanations, especially when the answers themselves were wrong. For example, if the 'secret image' portrays a dog, but the AI answers 'it's a surfer,' a visual explanation could help a human user realise the AI's mistake. According to the researchers, this proves that their game is a suitable tool for evaluating the helpfulness of AI explanations.

AMT Worker: What is in the image? VQA Ans: Toilet

Selected ✅

what kind of motorcycle is this?
Ans: harley

what is the number on the
motorcycle?
Ans: 69

what brand of motorcycle is this?
Ans: harley

what brand is the motorcycle?
Ans: bmw

what color is the motorcycle?
Ans: black

where is the man in the picture?
Ans: bathroom

what is the man standing in?
Ans: bathtub

what is the man taking a picture
of ?
Ans: toilet

what is the man on
Ans: toilet

what is the man in blue doing?
Ans: taking picture

what is the picture of
Ans:tennis

what sport is being played
in the image Ans:tennis

what is this a picture of
Ans:tennis player

what kind of car is in the
picture
Ans:mercedes-benz

what is in the girl's hand
Ans:tennis racket

what is on top of the toilet?
Ans: toilet paper

what color is the toilet?
Ans: white

what is the toilet seat made of?
Ans: wood

what kind of car is in the
picture?
Ans: white

what color is the wall behind
the toilet?
Ans: white

what is the color of the toilet?
Ans: white

what is on top of the toilet?
Ans: toilet paper

what color is the toilet?
Ans: white

what is above the toilet?
Ans: window

is there food in the image?
Ans: no

The figure above shows a gameplay with explanations. The heatmap visual explanation highlights the regions in the images that lead to AI answers. With such an explanation, users gain understanding that AI systems may pick up objects that are not the main focus of the image in human's perspective when answering a general question like "what is in the image". This hints the user to ask follow-up questions and finally select the secret image correctly. GT means Ground Truth (i.e. the secret image), Selected is the image selected by the user after asking the questions and getting the answers and/or explanations. Credit: Ray et al.

"In my opinion, the most interesting result of our study is that users can use just a few good explanations to win games when the AI answers are mostly wrong," Ray said. "In contrast, for games with similar answer accuracy but without explanations, users blindly trust AI-generated answers and lose the game. This supports the importance of even a few good explanations for a human-AI collaborative systems, especially when the AI system is imperfect, which it is in most cases these days."

To explain this idea better, Ray offers the example of self-driving vehicles. Over the past few years, there has been much debate about their safety, also due to accidents that occurred while the vehicles were being tested. According to Ray, effective AI explanations could encourage greater trust in the safety of self-driving vehicles, as they would allow human drivers to identify problems beforehand and prevent accidents.

"For instance, let's assume that the AI system is experiencing trouble detecting the lanes reliably," Ray said. "Since the road is currently straight, without additional information, the user would be unable to tell whether the AI is failing. Even if he/she had some doubts, he/she would probably not do anything until the last moment, when the car has to take a turn, doesn't, and crashes, which would too late. In contrast, if a screen in the car showed explanations of how AI is perceiving the environment, such as heat maps, the user would be able to tell the AI's latent failure and take control of the wheel in advance."

The researchers found that useful explanations positively affected human users' performance in the image-guessing game. Their findings suggest that having at least one 'correct' explanation was significantly helpful, particularly in cases where the AI's answers to user questions were 'noisy' or poorly defined. Interestingly, players developed a preference for explanations over answers and often rated the AI explanations as 'helpful.'

"I think that while several lines of work tried to provide explanations for an AI system's outcomes or actions, ours is the first study to introduce a human and machine collaboration task to evaluate the effectiveness of AI explanations; thus, it brought a lot of insight into how AI explanations could enhance human-robot interactions," Yi Yao, a senior technical manager at SRI International who was involved in the study, told TechXplore.

The study carried out by Ray and his colleagues is one of the first to provide tangible evidence of the usefulness of AI explanations. The researchers hope that their research will ultimately inform the development of AI systems that can act rationally in society, thus connecting and relating better with humans.

According to Ray, AI systems that can clearly explain the reasoning and processes behind their actions would be a significant step forward in the development of intelligent machines. By effectively answering questions and rationalizing their decisions, these systems could foster a greater sense of trust in AI, as well as a deeper relationship with it.

"Many other companies, groups and research groups have been addressing explainable AI, and there have been many proposals of how to extend existing AI models and systems to provide explanations to users," said Giedrius Burachas, a senior computer scientist at SRI International and principal investigator behind the DARPA study that led to the development of the Guess Which game. "While there were lots of ideas generated, evidence that these ideas work was lacking, so one of the strong sides of our research is that it provides indisputable evidence that certain types of explanations are really very effective in improving the collaboration with the AI systems, but also in building trust in them."

Up until now, the work of Ray and his colleagues primarily focused on visual question answering (VQA) tasks, where users ask questions about images and an AI answers. They are now planning to continue their research into AI explanation techniques, applying these techniques to a broader scope of AI tasks.

"We will also continue developing protocols to evaluate the effectiveness of the AI-generated explanations with finer granularity (e.g. what explanation is more effective under what scenarios?) and from different perspectives (e.g. do explanations help users to build the mental model?)," Ray said. "To close the loop, we will use lessons learned from these evaluations to develop more effective explanation methods. We believe that the Holy Grail of explainable AI is to devise explanations that not only inform users but also improve machine performance by improving its reasoning ability."

In addition to exploring the effects of AI explanations on the performance and perceptions of human users, therefore, the researchers would like to investigate their impact on the AI systems

themselves. They feel that AI explanations could also make AI systems inherently better, as they would gradually acquire reasoning and rationalization skills. [25]

Inequalities in the UK can be detected using deep learning image analysis

Social, economic, environmental and health inequalities within cities can be detected using street imagery. The findings, from scientists at Imperial College London, are published in *Scientific Reports* this week.

Detailed measurements of the substantial inequalities that exist within large cities like London are crucial for informing and evaluating policies that aim to reduce them. However, only a small number of countries have fully linked statistical datasets that allow for real-time measurements.

Esra Suel and colleagues from Imperial's School of Public Health used a deep-learning approach to train a computer programme to detect inequalities in four major UK cities – London, Birmingham, Manchester and Leeds – using publicly available street view images and government statistics.

Trained on 156,581 images from London corresponding to 156,581 postcodes, the programme predicted outcomes with similar accuracy in the other three cities, after it had been fine-tuned with only 1% of additional images collected in the West Midlands, Greater Manchester and West Yorkshire.

The authors hypothesized that some features of cities and urban life, such as quality of housing and the living environment, have direct visual signals that a computer could recognize.

Local shops and disrepair

These visual signals include building materials and disrepair, cars, or local shops. Combined with government statistics on outcomes such as housing conditions, mean income, or mortality and morbidity rates for one city, images may be used to train a computer programme to detect inequalities in other cities that lack statistical data.

The authors found that their computer programme was most successful at recognizing differences in quality of the living environment and mean income.

'Measuring social, environmental and health inequalities using deep learning and street imagery' by E.Suel et al is published in the journal *Scientific Reports*. [24]

AI adjusts for gaps in citizen science data

Citizen science is a boon for researchers, providing reams of data about everything from animal species to distant galaxies.

But crowdsourced information can be inconsistent. More reports come from densely populated areas and fewer from spots that are hard to access, creating challenges for researchers who need evenly distributed data.

"There is a huge bias in the data set because the data is collected by volunteers," said Di Chen, a doctoral student in computer science and first author of "Bias Reduction via End to End Shift Learning: Application to Citizen Science," which will be presented at the AAAI Conference on Artificial Intelligence, Jan. 27-Feb. 1 in Honolulu.

"Since this is highly motivated by their personal interest, the distribution of this kind of data is not what scientists want," Chen said. "All the data is actually distributed along main roads and in urban areas because most people don't want to drive 200 miles to help us explore birds in a desert."

To compensate, Chen and Carla Gomes, professor of computer science and director of the Institute for Computational Sustainability, developed a deep learning model that effectively corrects for location biases in citizen science by comparing the population densities of various locations. Gomes and Chen tested their model on data from the Cornell Lab of Ornithology's eBird, which collects more than 100 million bird sightings submitted annually by birdwatchers worldwide.

"When I communicate with conservation biologists and ecologists, a big part of communicating about these estimates is convincing them that we are aware of these biases and, to the degree possible, controlling for them," said Daniel Fink, a senior research associate at the Lab of Ornithology who is collaborating with Gomes and Chen on this work. "This gives [biologists and ecologists] a better reason to trust these results and actually use them, and base decisions on them."

Researchers have long been aware of the problems with citizen science data and have tried various methods to address them, including other types of statistical models. Projects that offer incentives to entice volunteers to travel to remote spots or search for less-popular species have shown promise, but these can be expensive and hard to conduct on a large scale.

A massive data set like eBird's is useful in machine learning, where large amounts of data are used to train computers to make predictions and solve problems. But because of the location biases, a model created with the eBird data would make inaccurate predictions.

Adjusting for bias in the eBird data is further complicated by the data's many characteristics. Each bird sighting in the system comprises 16 distinct pieces of information, making it computationally challenging.

Chen and Gomes solved the problem using a deep learning model – a kind of artificial intelligence that is good at classifying – that adjusts for population differences in different areas by comparing their ratios of density.

"Right now the data we get is essentially biased because the birds don't just stay around cities, so we need to factor that in and correct that," Gomes said. "We need to make sure the training data is going to match what you would have in the real world."

Chen and Gomes tested several models and found their deep learning algorithm to be more effective than other statistical or machine learning models at predicting where bird species might be found.

Though they worked with eBird, their findings could be used in any kind of citizen science project, Gomes said.

"There are many, many applications that rely on citizen science, and this problem is prevalent, so you really need to correct for it, whether people are classifying birds, galaxies or other situations where data biases can skew the learned model," she said. [23]

Machine learning in action for the humanitarian sector

Governments across the world came together in Marrakesh this past December to ratify a pact to improve cooperation on international migration. Among other objectives, the Global Compact for Migration seeks to use "accurate and disaggregated data as a basis for evidence-based policies." How can machine learning technologies help with deeply polarizing societal issues like migration?

In early 2018, with support from IBM Corporate Citizenship and the Danish Ministry for Foreign Affairs, IBM and the Danish Refugee Council (DRC) embarked on a partnership aimed squarely at the need to better understand migration drivers and evidence-based policy guidance for a range of stakeholders. At the recent THINK Copenhagen keynote, the Secretary General of the DRC, Christian Friis Bach, presented the first results of this effort.

In this post, I'll walk through the development of a machine learning system that provides strategic forecasts of mixed migration along with scenario analysis. Mixed migration refers to cross-border movements of people that are motivated by a multiplicity of factors to move, including refugees fleeing persecution and conflict, victims of trafficking, and people seeking better lives and opportunity. Such populations have a range of legal statuses, some of which are not reflected in official government statistics.

Credit: IBM

Understanding migration dynamics and drivers is inherently complex. Circumstances differ from person to person. The question "why did you decide to move?" is not straightforward for people to answer. However, to the extent that individual decisions reflect structural societal factors, the dynamics can be partially explained by aggregate measures. For instance, economic drivers for movement can be expected to be related to employment opportunities and therefore macro indicators on employment. These challenges are compounded by data availability and coverage on specific indicators.

The forecasting system

We started by leveraging the 4MI monitoring program run by the DRC through which thousands of migrants on the move are interviewed. Analysis of survey data reveals high-level clusters of drivers for migration. These clusters ranged from lack of rights and other social services, to economic necessity and conflict. These drivers are then mapped to quantitative indicators. Features derived from these indicators are then fed to a model that generates forecasts along with confidence

intervals (Figure 1). In addition, the system also generates context for each prediction by showing specific drivers that contributed to the forecast.

Using these indicators, we developed an ensemble model to make strategic forecasts annually for bilateral flows on mixed-migration volumes annually. Our evaluations showing error rates to be within a few thousand persons per year even for countries with volatile conditions. The system further allows for scenario analysis, where relative changes in influencing factors can be modelled to make adjusted predictions.

Interesting counter-intuitive dynamics emerge from such analysis. For instance, unemployment rates in Ethiopia are above average compared to Sub-Saharan countries. A large number of Ethiopians travel to Saudi Arabia for work. Increases in employment rates to the best fifth in the region will result in greater migration to the UK (two percent increase), Sweden (two percent increase) and Saudi Arabia (eight percent increase). This reflects an increased ability and means of Ethiopians to meet their aspirations abroad. If unemployment increases to the worst levels, the model predicts an increase of migration to South Africa (three percent increase) and Saudi Arabia (four percent increase), with EU destinations largely invariant to increases in unemployment.
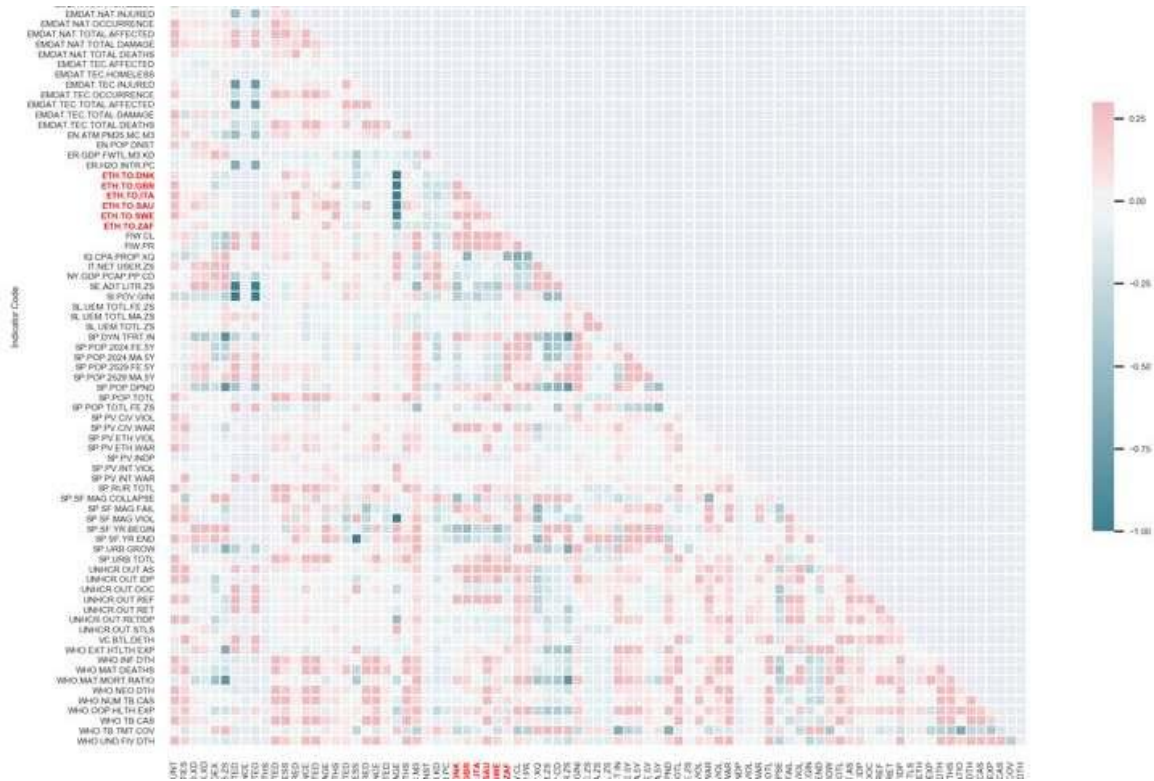

Figure 2: Correlation matrix for all features considered in the model (no temporal effects). Credit: IBM

Such detailed quantitative analysis has previously not been available to stakeholders who need to formulate policy responses.

Causal inference

The forecasting system described above is purely data-driven where we rely on the model to derive relationships between all the variables. Alternatively, if we seek to exploit subject matter expertise and include specific insights in the system, we could take the approach of probabilistic graphical models.

At a workshop held at IBM Research – Ireland, subject matter experts from the Mixed Migration Centre in Geneva and DRC drew out the "spaghetti" network showing how they expect indicator clusters to be causally linked. Using this as input, we then combined their expert opinion with the data. We used a technique called structure learning to develop such a network.

Forecasting using such networks typically don't perform as well as purely data-driven approaches presented above; nevertheless, they do aid in scenario analysis and policy analysis.

What's next?
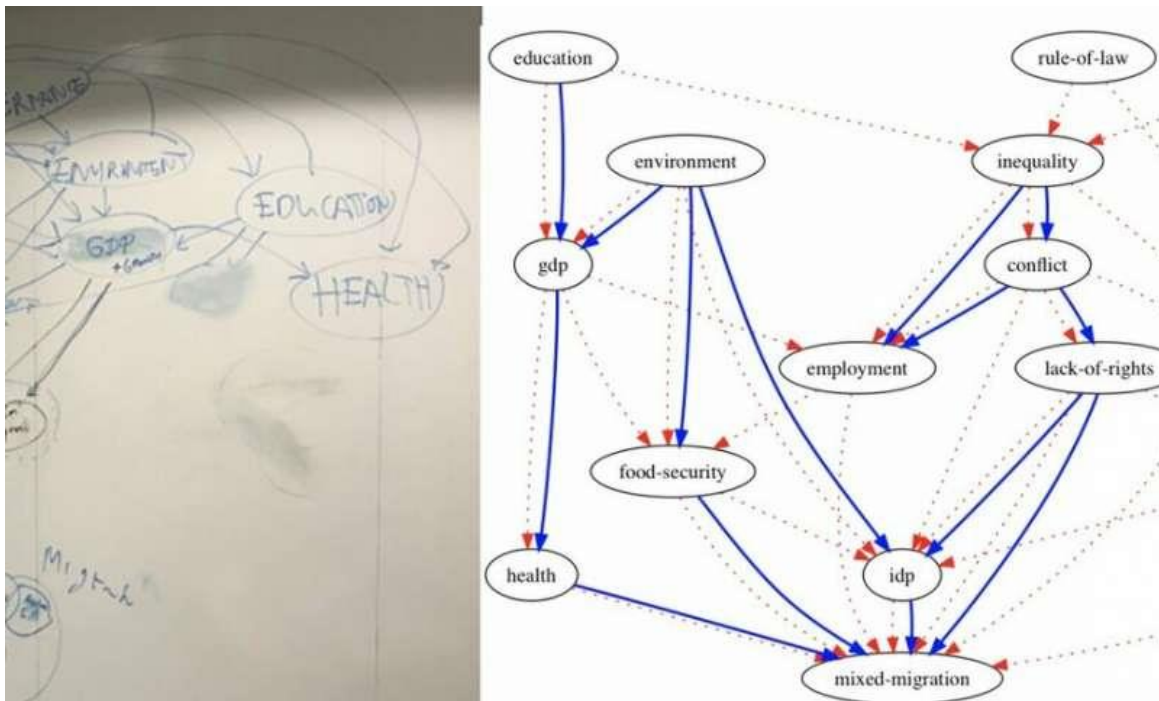
Figure 3: (left) causal network drawn by experts and (right) network learnt based on expert opinion and evidence based on data for all of Sub-Saharan Africa. Credit: IBM

These are the first few steps towards a future where policy makers have instant access to evidence when and where it is needed and where complex relationships can be explored easily to provide more insight driving better policy.

For now, we are continuing to improve the system and gather user feedback with subject experts within the DRC. Following more detailed validation, we will look to expand the geographic scope and scenario analysis capabilities. [22]

Machine learning technique to predict human cell organization published in nature methods

Scientists at the Allen Institute have used machine learning to train computers to see parts of the cell the human eye cannot easily distinguish. Using 3-D images of fluorescently labeled cells, the research team taught computers to find structures inside living cells without fluorescent labels, using only black and white images generated by an inexpensive technique known as brightfield microscopy. A study describing the new technique is published today in the journal *Nature Methods*.

Fluorescence microscopy, which uses glowing molecular labels to pinpoint specific parts of cells, is very precise but only allows scientists to see a few structures in the cell at a time. Human cells have upwards of 20,000 different proteins that, if viewed together, could reveal important information about both healthy and diseased cells.

"This technology lets us view a larger set of those structures than was possible before," said Greg Johnson, Ph.D., Scientist at the Allen Institute for Cell Science, a division of the Allen Institute, and senior author on the study. "This means that we can explore the organization of the cell in ways that nobody has been able to do, especially in live cells."

The prediction tool could also help scientists understand what goes wrong in cells during disease, said Rick Horwitz, Ph.D., Executive Director of the Allen Institute for Cell Science. Cancer researchers could potentially apply the technique to archived tumor biopsy samples to better understand how cellular structures change as cancers progress or respond to treatment. The algorithm could also aid regeneration medicine by uncovering how cells change in real time as scientists attempt to grow organs or other new body structures in the lab.

"This technique has huge potential ramifications for these and related fields," Horwitz said. "You can watch processes live as they are taking place—it's almost like magic. This method allows us, in the most non-invasive way that we have so far, to obtain information about human cells that we were previously unable to get."

The combination of the freely available prediction toolset and brightfield microscopy could lower research costs if used in place of fluorescence microscopy, which requires expensive equipment and trained operators. Fluorescent tags are also subject to fading, and the light itself can damage living cells, limiting the technique's utility to study live cells and their dynamics. The machine learning approach would allow scientists to track precise changes in cells over long periods of time, potentially shedding light on events such as early development or disease progression.

To the human eye, cells viewed in a brightfield microscope are sacs rendered in shades of gray. A trained scientist can find the edges of a cell and the nucleus, the cell's DNA-storage compartment, but not much else. The research team used an existing machine learning technique, known as a convolutional neural network, to train computers to recognize finer details in these images, such as the mitochondria, cells' powerhouses. They tested 12 different cellular structures and the model

generated predicted images that matched the fluorescently labeled images for most of those structures, the researchers said.

It also turned out what the algorithm was able to capture surprised even the modeling scientists.

"Going in, we had this idea that if our own eyes aren't able to see a certain structure, then the machine wouldn't be able to learn it," said Molly Maleckar, Ph.D., Director of Modeling at the Allen Institute for Cell Science and an author on the study. "Machines can see things we can't. They can learn things we can't. And they can do it much faster."

The technique can also predict precise structural information from images taken with an electron microscope. The computational approach here is the same, said Forrest Collman, Ph.D., Assistant Investigator at the Allen Institute for Brain Science and an author on the study, but the applications are different. Collman is part of a team working to map connections between neurons in the mouse brain. They are using the method to line up images of the neurons taken with different types of microscopes, normally a challenging problem for a computer and a laborious task for a human.

"Our progress in tackling this problem was accelerated by having our colleagues from the Allen Institute for Cell Science working with us on the solution," Collman said.

Roger Brent, Ph.D., a Member of the Basic Sciences Division at Fred Hutchinson Cancer Research Center, is using the new approach as part of a research effort he is leading to improve the "seeing power" of microscopes for biologists studying yeast and mammalian cells. "Replacing fluorescence microscopes with less light intensive microscopes would enable researchers to accelerate their work, make better measurements of cell and tissue function, and save some money in the process," Brent said. "By making these networks available, the Allen Institute is helping to democratize biological and medical research." [21]

Machine learning classifies biomolecules

Small angle X-ray scattering (SAXS) is one of a number of biophysical techniques used for determining the structural characteristics of biomolecules. Daniel Franke and colleagues from the European Molecular Biology Laboratory have recently published a machine learning-based method to classify biomolecules using existing SAXS data (*Biophys. J.* **114** 2485).

The method can be used to classify shape, as well as estimate structural parameters such as the maximal diameter or molecular mass of the molecule under study. These estimates may then serve as a valuable method for validating expected values.

The team decided on a set of shape classifications for biomolecules: compact spheres, flat discs, extended rods, compact-hollow cylinders, hollow spheres and flat rings. They used simulations to obtain idealized scattering profiles of each of these different geometries across a range of heights, widths and lengths ranging from 10 to 500 Å.
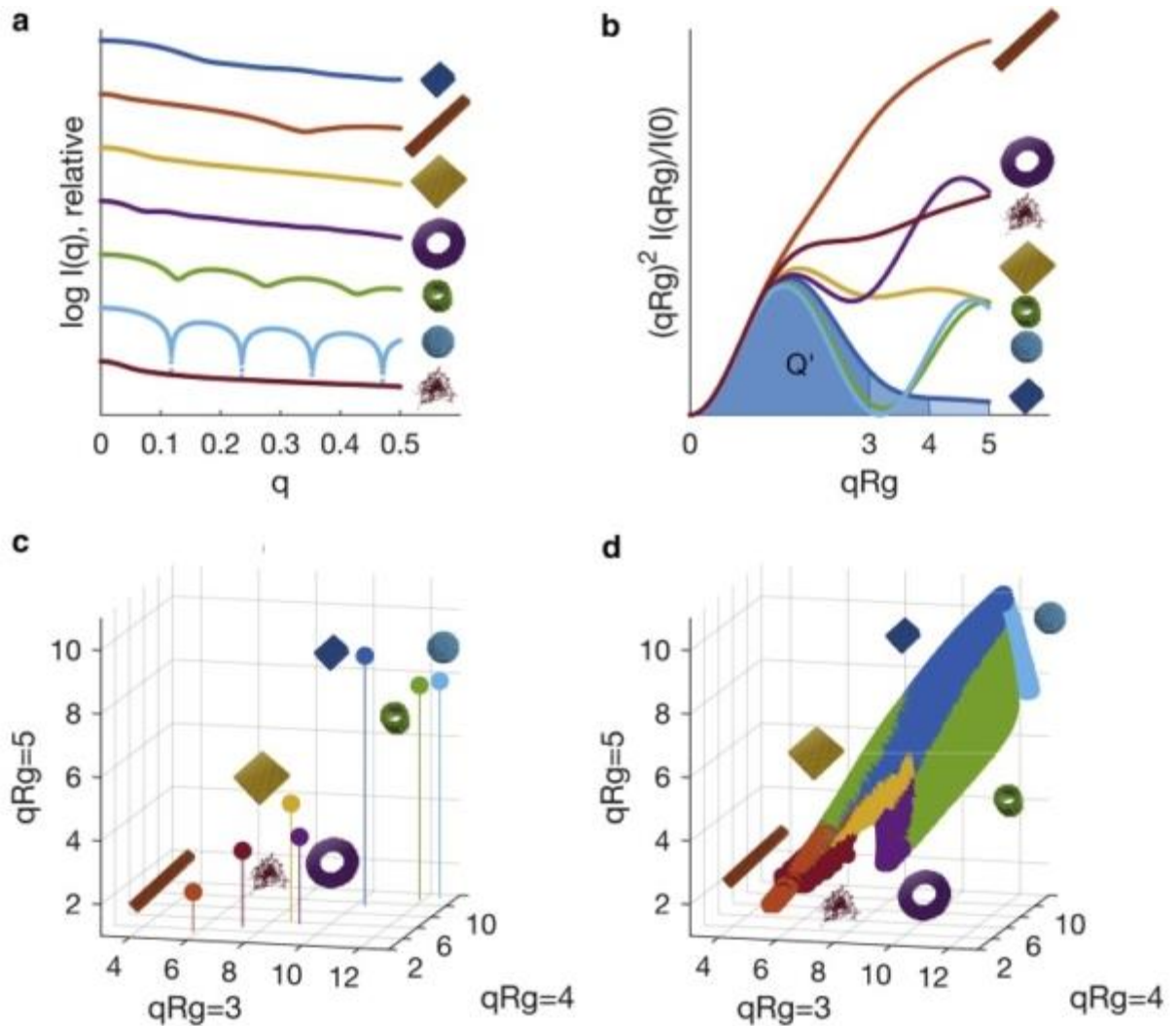
Simulated scattering intensity profiles for different molecular shape classes, shown schematically on the right (a). Reduced form of the intensity profile for each shape class (b). Each shape class defines a point cloud in normalized apparent volume space, with each shape falling into well-defined regions (c, d). (Courtesy: Franke et al Biophys. J. 114 2485 ©2018, with permission from Elsevier)

The researchers used innovative data reduction approaches to reduce each of the scattering profiles to a point in normalized apparent volume space, V. Representing the data in this way is advantageous because structures that share similar structural characteristics will occupy a similar position in V space.

The process of classifying an unknown scattering profile then amounts to calculating its position in V space and locating the nearest points in V space for which parameters are already known. The new parameters can then be estimated by taking a weighted average of these "nearest neighbour" points in V space. A machine can be programmed to perform all of these steps.

Using machine learning

The team simulated some 488,000 scattering patterns and used these to train an algorithm to categorize different scattering patterns. Each scattering pattern was then removed in turn, and the remaining data used to predict the shape classification of the removed pattern.

This training procedure allowed the researchers to refine the weights assigned to the nearest neighbour structures in V space, so as to maximize the accuracy of the machine classification.

Predicting structural parameters

To test the predictive power of the shape classification method, the researchers harvested scattering data from the Protein Data Bank (PDB) and the Small Angle Scattering Biological Data Bank (SASBDB).

From the atomic structures stored in the PDB, they used CRYSOL software to generate scattering intensities, as well as values of structural parameters such as the maximal diameter and molecular mass. After mapping the known structures to V space, an equivalent algorithm was then used to predict the structural parameters based on the generated scattering intensity. Here, the machine prediction was within 10% of the expected value in 90% of cases.

The SASBDB provides scattering intensity as well as user generated values of structural parameters such as the maximal diameter. The researchers also observed good agreement from the structures collected from the SASBDB, with the machine predicting a small, systematically lower value for the maximal diameter. This offset reflects the fact that molecules tend to occupy an extended configuration in solution.

The protocol developed by the team shows that data mining has significant potential to increase the efficiency and reliability of scattering data, which could have huge benefit for the biophysics community. [20]

Enhanced detection of nuclear events, thanks to deep learning

A deep neural network running on an ordinary desktop computer is interpreting highly technical data related to national security as well as—and sometimes better than—today's best automated methods or even human experts.

The progress tackling some of the most complex problems of the environment, the cosmos and national security comes from scientists at the Department of Energy's Pacific Northwest National Laboratory who presented their work at the 11th MARC conference—Methods and Applications of Radioanalytical Chemistry—in April in Hawaii. Their work employs deep learning, in which machines are enabled to learn and make decisions without being explicitly programmed for all conditions.

The research probes incredibly complex data sets from the laboratory's shallow underground lab, where scientists detect the faintest of signals from a planet abuzz in activity. In the laboratory buried 81 feet beneath concrete, rock and earth, thick shielding dampens signals from cosmic rays,

electronics and other sources. That allows PNNL scientists to isolate and decipher signals of interest collected from anywhere on the planet.

Those signals signify events called radioactive decays, when a particle such as an electron is emitted from an atom. The process is happening constantly, through both natural and human activity. Scientists can monitor changes in levels of argon-37, which could indicate prior nuclear test activity, and argon-39, whose levels help scientists determine the age of groundwater and learn more about the planet.

The lab has accumulated data on millions of radioactive decay events since it opened in 2010. But it's a noisy world out there, especially for scientists listening for very rare signals that are easily confused with signals of a different and frequently routine origin—for instance, a person flipping on a light switch or receiving a call on a cell phone.

PNNL scientist Emily Mace, who presented at MARC, is an expert in interpreting the features of such signals—when an event might indicate underground nuclear testing, for example, or a rapidly depleting aquifer. Much like physicians peruse X-rays for hints of disease, Mace and her colleagues pore over radioactive decay event data regularly to interpret the signals—their energy, timing, peaks, slopes, duration, and other features.

"Some pulse shapes are difficult to interpret," said Mace. "It can be challenging to differentiate between good and bad data."

Recently Mace and colleagues turned for input to their colleagues who are experts in deep learning, an exciting and active subfield of artificial intelligence. Jesse Ward is one of dozens of deep learning experts at the lab who are exploring several applications through PNNL's Deep Learning for Scientific Discovery Agile Investment. Mace sent Ward information on nearly 2 million energy pulses detected in the Shallow Underground Laboratory since 2010.

Ward used a clean sample set of 32,000 pulses to train the network, inputting many features of each pulse and showing the network how the data was interpreted. Then he fed the network thousands more signals as it taught itself to differentiate between "good" signals that showed something of interest and "bad" signals that amounted to unwanted noise. Finally, he tested the network, feeding it increasingly complex sets of data that are difficult even for experts to interpret.

The network he created interprets pulse shape events with an accuracy that equals and sometimes surpasses the know-how of experts like Mace. With straightforward data, the program sorted more than 99.9 percent of the pulses correctly.

Results are even more impressive when the data is noisy and includes an avalanche of spurious signals:

In an analysis involving 50,000 pulses, the neural network agreed 100 percent of the time with the human expert, besting the best conventional computerized techniques which agreed with the expert 99.8 percent of the time.

In another analysis of 10,000 pulses, the neural net correctly identified 99.9 percent of pulses compared to 96.1 percent with the conventional technique. Included in this analysis were the

toughest pulses to interpret; with that subset, the neural network did more than 25 times better, correctly classifying 386 out of 400 pulses compared to 14 of 400 for the conventional technique.

"This is a relatively simple neural network but the results are impressive," said Ward. "You can do productive work on important scientific problems with a fairly primitive machine. It's exciting to consider what else is possible."

The project posed an unexpected challenge, however: The shallow underground lab is so pristine, with most spurious noise signals mitigated before they enter the data stream, that Ward found himself asking Mace for more bad data.

"Signals can be well behaved or they can be poorly behaved," said Ward. "For the network to learn about the good signals, it needs a decent amount of bad signals for comparison."

The problem of culling through vast amounts of data looking for meaningful signals has a raft of implications and extends to many areas of science. At PNNL, one area is the search for signals that would result from dark matter, the vast portion of matter in our universe whose origin and whereabouts is unknown. Another is the automatic detection of breast cancers and other tissue anomalies.

"Deep learning is making it easier for us to filter out a small number of good events that are indicative of the activity of interest," said Craig Aalseth, nuclear physicist and PNNL laboratory fellow. "It's great to see deep-learning techniques actually doing a better job than our previous best detection techniques." [19]

Scientists pioneer use of deep learning for real-time gravitational wave discovery

Scientists at the National Center for Supercomputing Applications (NCSA), located at the University of Illinois at Urbana-Champaign, have pioneered the use of GPU-accelerated deep learning for rapid detection and characterization of gravitational waves. This new approach will enable astronomers to study gravitational waves using minimal computational resources, reducing time to discovery and increasing the scientific reach of gravitational wave astrophysics. This innovative research was recently published in *Physics Letters B*.

Combining deep learning algorithms, numerical relativity simulations of black hole mergers—obtained with the Einstein Toolkit run on the Blue Waters supercomputer—and data from the LIGO Open Science Center, NCSA Gravity Group researchers Daniel George and Eliu Huerta produced Deep Filtering, an end-to-end time-series signal processing method. Deep Filtering achieves similar sensitivities and lower errors compared to established gravitational wave detection algorithms, while being far more computationally efficient and more resilient to noise anomalies. The method allows faster than real-time processing of gravitational waves in LIGO's raw data, and also enables new physics, since it can detect new classes of gravitational wave sources that may go unnoticed

with existing detection algorithms. George and Huerta are extending this method to identify in real-time electromagnetic counterparts to gravitational wave events in future LSST data.

NCSA's Gravity Group leveraged NCSA resources from its Innovative Systems Laboratory, NCSA's Blue Waters supercomputer, and collaborated with talented interdisciplinary staff at the University of Illinois. Also critical to this research were the GPUs (Tesla P100 and DGX-1) provided by NVIDIA, which enabled an accelerated training of neural networks. Wolfram Research also played an important role, as the Wolfram Language was used in creating this framework for deep learning.

George and Huerta worked with NVIDIA and Wolfram researchers to create this demo to visualize the architecture of Deep Filtering, and to get insights into its neuronal activity during the detection and characterization of real gravitational wave events. This demo highlights all the components of Deep Filtering, exhibiting its detection sensitivity and computational performance. [18]

## Mathematicians develop model for how new ideas emerge

Researchers from Queen Mary University of London have developed a mathematical model for the emergence of innovations.

Studying creative processes and understanding how innovations arise and how novelties can trigger further discoveries could lead to effective interventions to nurture the success and sustainable growth of society.

Empirical findings have shown that the way in which novelties are discovered follows similar patterns in a variety of different contexts including science, arts, and technology.

The study, published in *Physical Review Letters*, introduces a new mathematical framework that correctly reproduces the rate at which novelties emerge in real systems, known as Heaps' law, and can explain why discoveries are strongly correlated and often come in clusters.

It does this by translating the theory of the 'adjacent possible', initially formulated by Stuart Kauffman in the context of biological systems, into the language of complex networks. The adjacent possible is the set of all novel opportunities that open up when a new discovery is made. Networks have emerged as a powerful way to both investigate real world systems, by capturing the essential relations between the components, and to model the hidden structure behind many complex social phenomena.
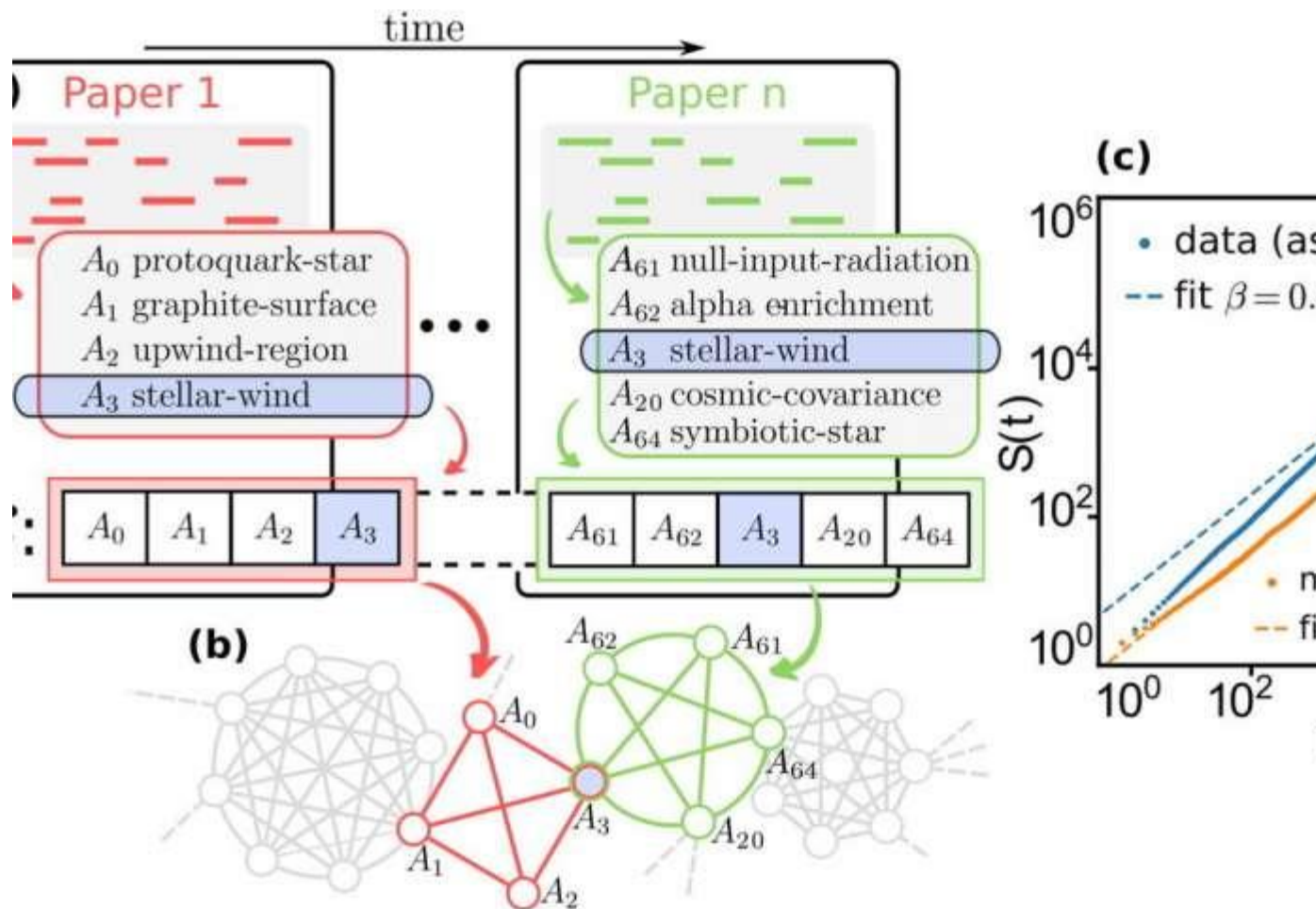
Growth of knowledge in science. (a) An empirical sequence of scientific concepts S is extracted from a temporally ordered sequence of papers by concatenating, for each scientific field, the relevant concepts present in the abstracts. (b) …more

In this work, networks are used to model the underlying space of relations among concepts.

Lead author Professor Vito Latora, from Queen Mary's School of Mathematical Sciences, said: "This research opens up new directions for the modelling of innovation, together with a new framework that could become important in the investigation of technological, biological, artistic, and commercial systems."

He added: "Studying the processes through which innovations arise can help understanding the main ingredients behind a winning idea, a breakthrough technology or a successful commercial activity, and is fundamental to devise effective data-informed decisions, strategies, and interventions to nurture the success and sustainable growth of our society."

In the study, the discovery process is modelled as a particular class of random walks, named 'reinforced' walks, on an underlying network of relations among concepts and ideas. An innovation corresponds to the first visit of a site of the network, and every time a walker moves from a concept to another, such association (an edge in the network) is reinforced so that it will be used more frequently in the future. The researchers named this the 'edge-reinforced random walk' model.

To show how the model works in a real case, they also constructed a dataset of 20 years of scientific publications in different disciplines, such as astronomy, ecology, economics and mathematics to analyse the appearance of new concepts. This showed that, despite its simplicity, the edge-reinforced random walk model is able to reproduce how knowledge grows in modern science.

Professor Vito Latora added: "The framework we present constitutes a new approach for the study of discovery processes, in particular those for which the underlying network can be directly reconstructed from empirical data, for example users listening to music over a similarity network between songs. We are already working on this idea, together with an extended version of our model, where we study the collective exploration of these networked spaces by considering multiple walkers at the same time." [17]

Rise of the quantum thinking machines

Quantum computers can be made to utilize effects such as quantum coherence and entanglement to accelerate machine learning.

Although we typically view information as being an abstract or virtual entity, information, of course, must be stored in a physical medium. Information processing devices such as computers and phones are therefore fundamentally governed by the laws of physics. In this way, the fundamental physical limits of an agent's ability to learn are governed by the laws of physics. The best known theory of physics is quantum theory, which ultimately must be used to determine the absolute physical limits of a machine's ability to learn.

A quantum algorithm is a stepwise procedure performed on a quantum computer to solve a problem such as searching a database. Quantum machine learning software makes use of quantum algorithms to process information in ways that classical computers cannot. These quantum effects open up exciting new avenues which can, in principle, outperform the best known classical algorithms when solving certain machine learning problems. This is known as quantum enhanced machine learning.

Machine learning methods use mathematical algorithms to search for certain patterns in large data sets. Machine learning is widely used in biotechnology, pharmaceuticals, particle physics and many other fields. Thanks to the ability to adapt to new data, machine learning greatly exceeds the ability of people. Despite this, machine learning cannot cope with certain difficult tasks.

Quantum enhancement is predicted to be possible for a host of machine learning tasks, ranging from optimization to quantum enhanced deep learning.

In the new paper published in Nature, a group of scientists led by Skoltech Associate Professor Jacob Biamonte produced a feasibility analysis outlining what steps can be taken for practical quantum enhanced machine learning.

The prospects of using quantum computers to accelerate machine learning has generated recent excitement due to the increasing capabilities of quantum computers. This includes a commercially

available 2000 spin quantum accelerated annealing by the Canada-based company D-Wave Systems Inc. and a 16 qubit universal quantum processor by IBM which is accessible via a (currently free) cloud service.

The availability of these devices has led to increased interest from the machine learning community. The interest comes as a bit of a shock to the traditional quantum physics community, in which researchers have thought that the primary applications of quantum computers would be using quantum computers to simulate chemical physics, which can be used in the pharmaceutical industry for drug discovery. However, certain quantum systems can be mapped to certain machine learning models, particularly deep learning models. Quantum machine learning can be used to work in tandem with these existing methods for quantum chemical emulation, leading to even greater capabilities for a new era of quantum technology.

"Early on, the team burned the midnight oil over Skype, debating what the field even was—our synthesis will hopefully solidify topical importance. We submitted our draft to Nature, going forward subject to significant changes. All in all, we ended up writing three versions over eight months with nothing more than the title in common," said lead study author Biamonte. [16]

A Machine Learning Systems That Called Neural Networks Perform Tasks by Analyzing Huge Volumes of Data

Neural networks learn how to carry out certain tasks by analyzing large amounts of data displayed to them. These machine learning systems continually learn and readjust to be able to carry out the task set out before them. Understanding how neural networks work helps researchers to develop better applications and uses for them.

At the 2017 Conference on Empirical Methods on Natural Language Processing earlier this month, MIT researchers demonstrated a new general-purpose technique for making sense of neural networks that are able to carry out natural language processing tasks where they attempt to extract data written in normal text opposed to something of a structured language like database-query language.

The new technique works great in any system that reads the text as input and produces symbols as the output. One such example of this can be seen in an automatic translator. It works without the need to access any underlying software too. Tommi Jaakkola is Professor of Electrical Engineering and Computer Science at MIT and one of the authors on the paper. He says, "I can't just do a simple randomization. And what you are predicting is now a more complex object, like a sentence, so what does it mean to give an explanation?"

As part of the research, Jaakkola, and colleague David Alvarez-Melis, an MIT graduate student in electrical engineering and computer science and first author on the paper, used a black-box neural net in which to generate test sentences to feed black-box neural nets. The duo began by teaching the network to compress and decompress natural sentences. As the training continues the encoder and decoder get evaluated simultaneously depending on how closely the decoder's output matches up with the encoder's input.

Neural nets work on probabilities. For example, an object-recognition system could be fed an image of a cat, and it would process that image as it saying 75 percent probability of being a cat, while still having a 25 percent probability that it's a dog. Along with that same line, Jaakkola and Alvarez-Melis' sentence compressing network has alternative words for each of those in a decoded sentence along with the probability that each is correct. So, once the system has generated a list of closely related sentences they're then fed to a black-box natural language processor. This then allows the researchers to analyze and determine which inputs have an effect on which outputs.

During the research, the pair applied this technique to three different types of a natural language processing system. The first one inferred the way in which words were pronounced; the second was a set of translators, and the third was a simple computer dialogue system which tried to provide adequate responses to questions or remarks. In looking at the results, it was clear and pretty obvious that the translation systems had strong dependencies on individual words of both the input and output sentences. A little more surprising, however, was the identification of gender biases in the texts on which the machine translation systems were trained. The dialogue system was too small to take advantage of the training set.

"The other experiment we do is in flawed systems," says Alvarez-Melis. "If you have a black-box model that is not doing a good job, can you first use this kind of approach to identify problems? A motivating application of this kind of interpretability is to fix systems, to improve systems, by understanding what they're getting wrong and why." [15]

Active machine learning for the discovery and crystallization of gigantic polyoxometalate molecules

Who is the better experimentalist, a human or a robot? When it comes to exploring synthetic and crystallization conditions for inorganic gigantic molecules, actively learning machines are clearly ahead, as demonstrated by British Scientists in an experiment with polyoxometalates published in the journal Angewandte Chemie.

Polyoxometalates form through self-assembly of a large number of metal atoms bridged by oxygen atoms. Potential uses include catalysis, electronics, and medicine. Insights into the self-organization processes could also be of use in developing functional chemical systems like "molecular machines".

Polyoxometalates offer a nearly unlimited variety of structures. However, it is not easy to find new ones, because the aggregation of complex inorganic molecules to gigantic molecules is a process that is difficult to predict. It is necessary to find conditions under which the building blocks aggregate and then also crystallize, so that they can be characterized.

A team led by Leroy Cronin at the University of Glasgow (UK) has now developed a new approach to define the range of suitable conditions for the synthesis and crystallization of polyoxometalates. It is based on recent advances in machine learning, known as active learning. They allowed their trained machine to compete against the intuition of experienced experimenters. The test example was $Na_6[Mo_{120}Ce_6O_{366}H_{12}(H_2O)_{78}]\cdot200\ H_2O$, a new, ring-shaped polyoxometalate cluster that was recently discovered by the researchers' automated chemical robot.

In the experiment, the relative quantities of the three necessary reagent solutions were to be varied while the protocol was otherwise prescribed. The starting point was a set of data from successful and unsuccessful crystallization experiments. The aim was to plan ten experiments and then use the results from these to proceed to the next set of ten experiments - a total of one hundred crystallization attempts.

Although the flesh-and-blood experimenters were able to produce more successful crystallizations, the far more "adventurous" machine algorithm was superior on balance because it covered a significantly broader domain of the "crystallization space". The quality of the prediction of whether an experiment would lead to crystallization was improved significantly more by the machine than the human experimenters. A series of 100 purely random experiments resulted in no improvement. In addition, the machine discovered a range of conditions that led to crystals which would not have been expected based on pure intuition. This "unbiased" automated method makes the discovery of novel compounds more probably than reliance on human intuition. The researchers are now looking for ways to make especially efficient "teams" of man and machine. [14]

Using machine learning to understand materials

Whether you realize it or not, machine learning is making your online experience more efficient. The technology, designed by computer scientists, is used to better understand, analyze, and categorize data. When you tag your friend on Facebook, clear your spam filter, or click on a suggested YouTube video, you're benefitting from machine learning algorithms.

Machine learning algorithms are designed to improve as they encounter more data, making them a versatile technology for understanding large sets of photos such as those accessible from Google Images. Elizabeth Holm, professor of materials science and engineering at Carnegie Mellon University, is leveraging this technology to better understand the enormous number of research images accumulated in the field of materials science. This unique application is an interdisciplinary approach to machine learning that hasn't been explored before.

"Just like you might search for cute cat pictures on the internet, or Facebook recognizes the faces of your friends, we are creating a system that allows a computer to automatically understand the visual data of materials science," explains Holm.

The field of materials science usually relies on human experts to identify research images by hand. Using machine learning algorithms, Holm and her group have created a system that automatically recognizes and categorizes microstructural images of materials. Her goal is to make it more efficient for materials scientists to search, sort, classify, and identify important information in their visual data.

"In materials science, one of our fundamental data is pictures," explains Holm. "Images contain information that we recognize, even when we find it difficult to quantify numerically."

Holm's machine learning system has several different applications within the materials science field including research, industry, publishing, and academia. For example, the system could be used to create a visual search of a scientific journal archives so that a researcher could find out whether a similar image had ever been published. Similarly, the system can be used to automatically search

and categorize image archives in industries or research labs. "Big companies can have archives of 600,000 or more research images. No one wants to look through those, but they want to use that data to better understand their products," explains Holm. "This system has the power to unlock those archives."

Holm and her group have been working on this research for about three years and are continuing to grow the project, especially as it relates to the metal 3-D printing field. For example, they are beginning to compile a database of experimental and simulated metal powder micrographs in order to better understand what types of raw materials are best suited for 3-D printing processes.

Holm published an article about this research in the December 2015 issue of Computational Materials Science titled "A computer vision approach for automated analysis and classification of microstructural image data." [13]

Artificial intelligence helps in the discovery of new materials

With the help of artificial intelligence, chemists from the University of Basel in Switzerland have computed the characteristics of about two million crystals made up of four chemical elements. The researchers were able to identify 90 previously unknown thermodynamically stable crystals that can be regarded as new materials.

They report on their findings in the scientific journal Physical Review Letters.

Elpasolite is a glassy, transparent, shiny and soft mineral with a cubic crystal structure. First discovered in El Paso County (Colorado, USA), it can also be found in the Rocky Mountains, Virginia and the Apennines (Italy). In experimental databases, elpasolite is one of the most frequently found quaternary crystals (crystals made up of four chemical elements). Depending on its composition, it can be a metallic conductor, a semi-conductor or an insulator, and may also emit light when exposed to radiation.

These characteristics make elpasolite an interesting candidate for use in scintillators (certain aspects of which can already be demonstrated) and other applications. Its chemical complexity means that, mathematically speaking, it is practically impossible to use quantum mechanics to predict every theoretically viable combination of the four elements in the structure of elpasolite.

Machine learning aids statistical analysis

Thanks to modern artificial intelligence, Felix Faber, a doctoral student in Prof. Anatole von Lilienfeld's group at the University of Basel's Department of Chemistry, has now succeeded in solving this material design problem. First, using quantum mechanics, he generated predictions for thousands of elpasolite crystals with randomly determined chemical compositions. He then used the results to train statistical machine learning models (ML models). The improved algorithmic strategy achieved a predictive accuracy equivalent to that of standard quantum mechanical approaches.

ML models have the advantage of being several orders of magnitude quicker than corresponding quantum mechanical calculations. Within a day, the ML model was able to predict the formation energy – an indicator of chemical stability – of all two million elpasolite crystals that theoretically

can be obtained from the main group elements of the periodic table. In contrast, performance of the calculations by quantum mechanical means would have taken a supercomputer more than 20 million hours.

Unknown materials with interesting characteristics

An analysis of the characteristics computed by the model offers new insights into this class of materials. The researchers were able to detect basic trends in formation energy and identify 90 previously unknown crystals that should be thermodynamically stable, according to quantum mechanical predictions.

On the basis of these potential characteristics, elpasolite has been entered into the Materials Project material database, which plays a key role in the Materials Genome Initiative. The initiative was launched by the US government in 2011 with the aim of using computational support to accelerate the discovery and the experimental synthesis of interesting new materials.

Some of the newly discovered elpasolite crystals display exotic electronic characteristics and unusual compositions. "The combination of artificial intelligence, big data, quantum mechanics and supercomputing opens up promising new avenues for deepening our understanding of materials and discovering new ones that we would not consider if we relied solely on human intuition," says study director von Lilienfeld. [12]

Physicists are putting themselves out of a job, using artificial intelligence to run a complex experiment

The experiment, developed by physicists from The Australian National University (ANU) and UNSW ADFA, created an extremely cold gas trapped in a laser beam, known as a Bose-Einstein condensate, replicating the experiment that won the 2001 Nobel Prize.

"I didn't expect the machine could learn to do the experiment itself, from scratch, in under an hour," said co-lead researcher Paul Wigley from the ANU Research School of Physics and Engineering.

"A simple computer program would have taken longer than the age of the Universe to run through all the combinations and work this out."

Bose-Einstein condensates are some of the coldest places in the Universe, far colder than outer space, typically less than a billionth of a degree above absolute zero.

They could be used for mineral exploration or navigation systems as they are extremely sensitive to external disturbances, which allows them to make very precise measurements such as tiny changes in the Earth's magnetic field or gravity.

The artificial intelligence system's ability to set itself up quickly every morning and compensate for any overnight fluctuations would make this fragile technology much more useful for field measurements, said co-lead researcher Dr Michael Hush from UNSW ADFA.

"You could make a working device to measure gravity that you could take in the back of a car, and the artificial intelligence would recalibrate and fix itself no matter what," he said.

"It's cheaper than taking a physicist everywhere with you."

The team cooled the gas to around 1 microkelvin, and then handed control of the three laser beams over to the artificial intelligence to cool the trapped gas down to nanokelvin.

Researchers were surprised by the methods the system came up with to ramp down the power of the lasers.

"It did things a person wouldn't guess, such as changing one laser's power up and down, and compensating with another," said Mr Wigley.

"It may be able to come up with complicated ways humans haven't thought of to get experiments colder and make measurements more precise.

The new technique will lead to bigger and better experiments, said Dr Hush.

"Next we plan to employ the artificial intelligence to build an even larger Bose-Einstein condensate faster than we've seen ever before," he said.

The research is published in the Nature group journal Scientific Reports. [11]

Quantum experiments designed by machines

The idea was developed when the physicists wanted to create new quantum states in the laboratory, but were unable to conceive of methods to do so. "After many unsuccessful attempts to come up with an experimental implementation, we came to the conclusion that our intuition about these phenomena seems to be wrong. We realized that in the end we were just trying random arrangements of quantum building blocks. And that is what a computer can do as well - but thousands of times faster", explains Mario Krenn, PhD student in Anton Zeilinger's group and first author research.

After a few hours of calculation, their algorithm - which they call Melvin - found the recipe to the question they were unable to solve, and its structure surprised them. Zeilinger says: "Suppose I want build an experiment realizing a specific quantum state I am interested in. Then humans intuitively consider setups reflecting the symmetries of the state. Yet Melvin found out that the most simple realization can be asymmetric and therefore counterintuitive. A human would probably never come up with that solution."

The physicists applied the idea to several other questions and got dozens of new and surprising answers. "The solutions are difficult to understand, but we were able to extract some new experimental tricks we have not thought of before. Some of these computer-designed experiments are being built at the moment in our laboratories", says Krenn.

Melvin not only tries random arrangements of experimental components, but also learns from previous successful attempts, which significantly speeds up the discovery rate for more complex solutions. In the future, the authors want to apply their algorithm to even more general questions in quantum physics, and hope it helps to investigate new phenomena in laboratories. [10]

Moving electrons around loops with light: A quantum device based on geometry

Researchers at the University of Chicago's Institute for Molecular Engineering and the University of Konstanz have demonstrated the ability to generate a quantum logic operation, or rotation of the qubit, that - surprisingly—is intrinsically resilient to noise as well as to variations in the strength or duration of the control. Their achievement is based on a geometric concept known as the Berry phase and is implemented through entirely optical means within a single electronic spin in diamond.

Their findings were published online Feb. 15, 2016, in Nature Photonics and will appear in the March print issue. "We tend to view quantum operations as very fragile and susceptible to noise, especially when compared to conventional electronics," remarked David Awschalom, the Liew Family Professor of Molecular Engineering and senior scientist at Argonne National Laboratory, who led the research. "In contrast, our approach shows incredible resilience to external influences and fulfills a key requirement for any practical quantum technology."

Quantum geometry

When a quantum mechanical object, such as an electron, is cycled along some loop, it retains a memory of the path that it travelled, the Berry phase. To better understand this concept, the Foucault pendulum, a common staple of science museums helps to give some intuition. A pendulum, like those in a grandfather clock, typically oscillates back and forth within a fixed plane. However, a Foucault pendulum oscillates along a plane that gradually rotates over the course of a day due to Earth's rotation, and in turn knocks over a series of pins encircling the pendulum.

The number of knocked-over pins is a direct measure of the total angular shift of the pendulum's oscillation plane, its acquired geometric phase. Essentially, this shift is directly related to the location of the pendulum on Earth's surface as the rotation of Earth transports the pendulum along a specific closed path, its circle of latitude. While this angular shift depends on the particular path traveled, Awschalom said, it remarkably does not depend on the rotational speed of Earth or the oscillation frequency of the pendulum.

"Likewise, the Berry phase is a similar path-dependent rotation of the internal state of a quantum system, and it shows promise in quantum information processing as a robust means to manipulate qubit states," he said.

A light touch

In this experiment, the researchers manipulated the Berry phase of a quantum state within a nitrogen-vacancy (NV) center, an atomic-scale defect in diamond. Over the past decade and a half, its electronic spin state has garnered great interest as a potential qubit. In their experiments, the team members developed a method with which to draw paths for this defect's spin by varying the applied laser light. To demonstrate Berry phase, they traced loops similar to that of a tangerine slice within the quantum space of all of the potential combinations of spin states.

"Essentially, the area of the tangerine slice's peel that we drew dictated the amount of Berry phase that we were able to accumulate," said Christopher Yale, a postdoctoral scholar in Awschalom's laboratory, and one of the co-lead authors of the project.

This approach using laser light to fully control the path of the electronic spin is in contrast to more common techniques that control the NV center spin, through the application of microwave fields. Such an approach may one day be useful in developing photonic networks of these defects, linked and controlled entirely by light, as a way to both process and transmit quantum information.

A noisy path

A key feature of Berry phase that makes it a robust quantum logic operation is its resilience to noise sources. To test the robustness of their Berry phase operations, the researchers intentionally added noise to the laser light controlling the path. As a result, the spin state would travel along its intended path in an erratic fashion.

However, as long as the total area of the path remained the same, so did the Berry phase that they measured.

"In particular, we found the Berry phase to be insensitive to fluctuations in the intensity of the laser. Noise like this is normally a bane for quantum control," said Brian Zhou, a postdoctoral scholar in the group, and co-lead author.

"Imagine you're hiking along the shore of a lake, and even though you continually leave the path to go take pictures, you eventually finish hiking around the lake," said F. Joseph Heremans, co-lead author, and now a staff scientist at Argonne National Laboratory. "You've still hiked the entire loop regardless of the bizarre path you took, and so the area enclosed remains virtually the same."

These optically controlled Berry phases within diamond suggest a route toward robust and faulttolerant quantum information processing, noted Guido Burkard, professor of physics at the University of Konstanz and theory collaborator on the project.

"Though its technological applications are still nascent, Berry phases have a rich underlying mathematical framework that makes them a fascinating area of study," Burkard said. [9]

Researchers demonstrate 'quantum surrealism'

In a new version of an old experiment, CIFAR Senior Fellow Aephraim Steinberg (University of Toronto) and colleagues tracked the trajectories of photons as the particles traced a path through one of two slits and onto a screen. But the researchers went further, and observed the "nonlocal" influence of another photon that the first photon had been entangled with.

The results counter a long-standing criticism of an interpretation of quantum mechanics called the De Broglie-Bohm theory. Detractors of this interpretation had faulted it for failing to explain the behaviour of entangled photons realistically. For Steinberg, the results are important because they give us a way of visualizing quantum mechanics that's just as valid as the standard interpretation, and perhaps more intuitive.

"I'm less interested in focusing on the philosophical question of what's 'really' out there. I think the fruitful question is more down to earth. Rather than thinking about different metaphysical interpretations, I would phrase it in terms of having different pictures. Different pictures can be useful. They can help shape better intuitions."

At stake is what is "really" happening at the quantum level. The uncertainty principle tells us that we can never know both a particle's position and momentum with complete certainty. And when we do interact with a quantum system, for instance by measuring it, we disturb the system. So if we fire a photon at a screen and want to know where it will hit, we'll never know for sure exactly where it will hit or what path it will take to get there.

The standard interpretation of quantum mechanics holds that this uncertainty means that there is no "real" trajectory between the light source and the screen. The best we can do is to calculate a "wave function" that shows the odds of the photon being in any one place at any time, but won't tell us where it is until we make a measurement.

Yet another interpretation, called the De Broglie-Bohm theory, says that the photons do have real trajectories that are guided by a "pilot wave" that accompanies the particle. The wave is still probabilistic, but the particle takes a real trajectory from source to target. It doesn't simply "collapse" into a particular location once it's measured.

In 2011 Steinberg and his colleagues showed that they could follow trajectories for photons by subjecting many identical particles to measurements so weak that the particles were barely disturbed, and then averaging out the information. This method showed trajectories that looked similar to classical ones - say, those of balls flying through the air.

But critics had pointed out a problem with this viewpoint. Quantum mechanics also tells us that two particles can be entangled, so that a measurement of one particle affects the other. The critics complained that in some cases, a measurement of one particle would lead to an incorrect prediction of the trajectory of the entangled particle. They coined the term "surreal trajectories" to describe them.

In the most recent experiment, Steinberg and colleagues showed that the surrealism was a consequence of non-locality - the fact that the particles were able to influence one another instantaneously at a distance. In fact, the "incorrect" predictions of trajectories by the entangled photon were actually a consequence of where in their course the entangled particles were measured. Considering both particles together, the measurements made sense and were consistent with real trajectories.

Steinberg points out that both the standard interpretation of quantum mechanics and the De Broglie-Bohm interpretation are consistent with experimental evidence, and are mathematically equivalent. But it is helpful in some circumstances to visualize real trajectories, rather than wave function collapses, he says. [8]

Physicists discover easy way to measure entanglement—on a sphere
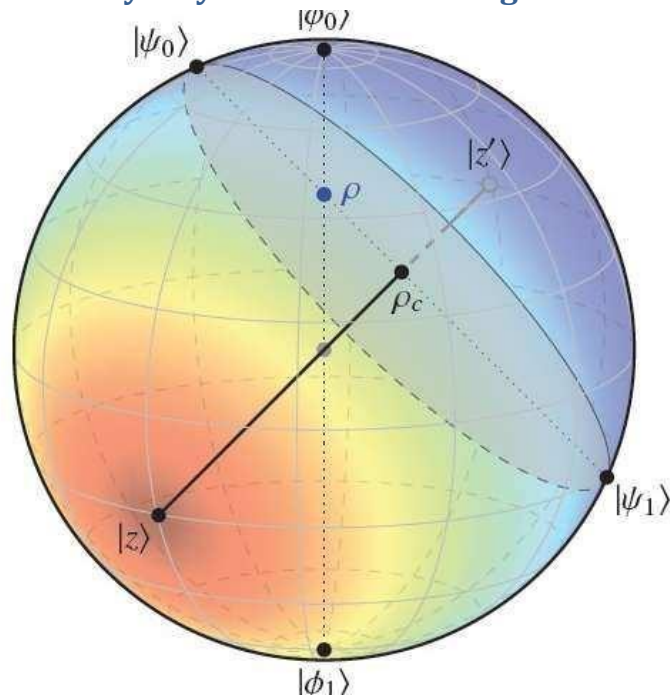
Entanglement on a sphere: This Bloch sphere shows entanglement for the one-root state ρ and its radial state ρ_c. The color on the sphere corresponds to the value of the entanglement, which is determined by the distance from the root state z, the point at which there is no entanglement. The closer to z, the less the entanglement (red); the further from z, the greater the entanglement (blue). Credit: Regula and Adesso. ©2016 American Physical Society

Now in a new paper to be published in Physical Review Letters, mathematical physicists Bartosz Regula and Gerardo Adesso at The University of Nottingham have greatly simplified the problem of measuring entanglement.

To do this, the scientists turned the difficult analytical problem into an easy geometrical one. They showed that, in many cases, the amount of entanglement between states corresponds to the distance between two points on a Bloch sphere, which is basically a normal 3D sphere that physicists use to model quantum states.

As the scientists explain, the traditionally difficult part of the math problem is that it requires finding the optimal decomposition of mixed states into pure states. The geometrical approach completely eliminates this requirement by reducing the many possible ways that states could decompose down to a single point on the sphere at which there is zero entanglement. The approach requires that there be only one such point, or "root," of zero entanglement, prompting the physicists to describe the method as "one root to rule them all."

The scientists explain that the "one root" property is common among quantum states and can be easily verified, transforming a formidable math problem into one that is trivially easy. They demonstrated that the new approach works for many types of two-, three- and four-qubit entangled states.

"This method reveals an intriguing and previously unexplored connection between the quantum features of a state and classical geometry, allowing all one-root states to enjoy a convenient visual representation which considerably simplifies the study and understanding of their properties," the researchers explained.

The simple way of measuring a state's entanglement could have applications in many technological areas, such as quantum cryptography, computation, and communication. It could also provide insight into understanding the foundations of thermodynamics, condensed matter physics, and biology. [7]

An idea for allowing the human eye to observe an instance of entanglement
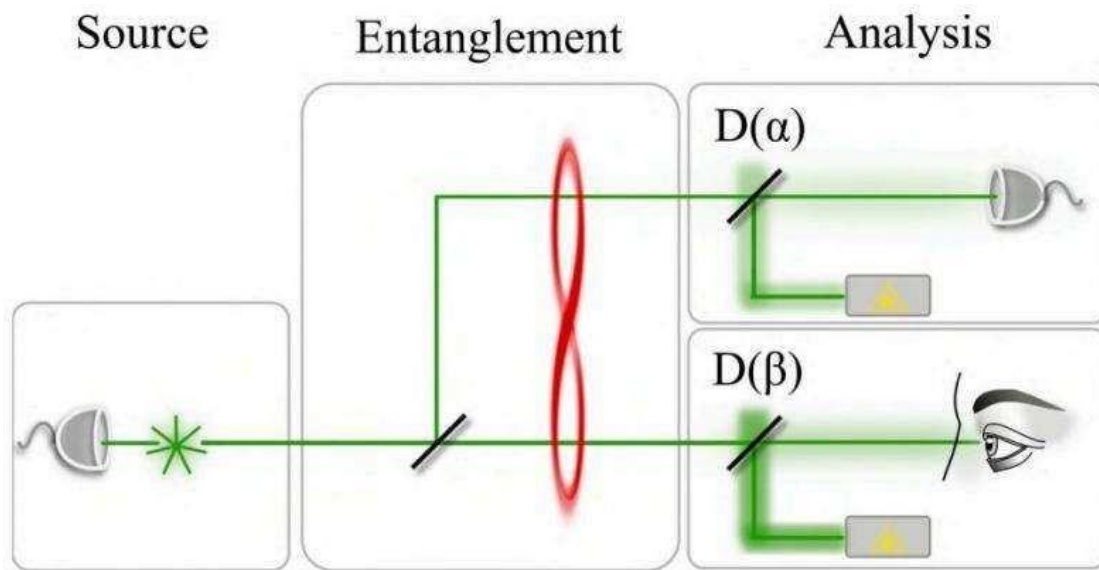
Scheme of the proposal for detecting entanglement with the human eye. Credit: arXiv:1602.01907

Entanglement, is of course, where two quantum particles are intrinsically linked to the extent that they actually share the same existence, even though they can be separated and moved apart. The idea was first proposed nearly a century ago, and it has not only been proven, but researchers routinely cause it to occur, but, to date, not one single person has every actually seen it happen—they only know it happens by conducting a series of experiments. It is not clear if anyone has ever actually tried to see it happen, but in this new effort, the research trio claim to have found a way to make it happen—if only someone else will carry out the experiment on a willing volunteer.

The idea involves using a beam splitter and two beans of light—an initial beam of coherent photons fired at the beam splitter and a secondary beam of coherent photons that interferes with the photons in the first beam causing a change of phase, forcing the light to be reflected rather than transmitted. In such a scenario, the secondary beam would not need to be as intense as the first, and could in fact be just a single coherent photon—if it were entangled, it could be used to allow a person to see the more powerful beam while still preserving the entanglement of the original photon.

The researchers suggest the technology to carry out such an experiment exists today, but also acknowledge that it would take a special person to volunteer for such an assignment because to prove that they had seen entanglement taking place would involve shooting a large number of photons in series, into a person's eye, whereby the resolute volunteer would announce whether they had seen the light on the order of thousands of times. [6]

Quantum entanglement

Measurements of physical properties such as position, momentum, spin, polarization, etc. performed on entangled particles are found to be appropriately correlated. For example, if a pair of particles is generated in such a way that their total spin is known to be zero, and one particle is found to have clockwise spin on a certain axis, then the spin of the other particle, measured on the same axis, will be found to be counterclockwise. Because of the nature of quantum measurement, however, this behavior gives rise to effects that can appear paradoxical: any measurement of a property of a particle can be seen as acting on that particle (e.g. by collapsing a number of superimposed states); and in the case of entangled particles, such action must be on the entangled system as a whole. It thus appears that one particle of an entangled pair "knows" what measurement has been performed on the other, and with what outcome, even though there is no known means for such information to be communicated between the particles, which at the time of measurement may be separated by arbitrarily large distances. [4]

The Bridge

The accelerating electrons explain not only the Maxwell Equations and the Special Relativity, but the Heisenberg Uncertainty Relation, the wave particle duality and the electron's spin also, building the bridge between the Classical and Quantum Theories. [1]

Accelerating charges

The moving charges are self maintain the electromagnetic field locally, causing their movement and this is the result of their acceleration under the force of this field. In the classical physics the charges will distributed along the electric current so that the electric potential lowering along the current, by linearly increasing the way they take every next time period because this accelerated motion. The same thing happens on the atomic scale giving a dp impulse difference and a dx way difference between the different part of the not point like particles.

Relativistic effect

Another bridge between the classical and quantum mechanics in the realm of relativity is that the charge distribution is lowering in the reference frame of the accelerating charges linearly: $ds/dt = at$ (time coordinate), but in the reference frame of the current it is parabolic: $s = a/2\ t^2$ (geometric coordinate).

Heisenberg Uncertainty Relation

In the atomic scale the Heisenberg uncertainty relation gives the same result, since the moving electron in the atom accelerating in the electric field of the proton, causing a charge distribution on delta x position difference and with a delta p momentum difference such a way that they product is about the half Planck reduced constant. For the proton this delta x much less in the nucleon, than in the orbit of the electron in the atom, the delta p is much higher because of the greater proton mass.

This means that the electron and proton are not point like particles, but has a real charge distribution.

Wave – Particle Duality

The accelerating electrons explains the wave – particle duality of the electrons and photons, since the elementary charges are distributed on delta x position with delta p impulse and creating a wave packet of the electron. The photon gives the electromagnetic particle of the mediating force of the electrons electromagnetic field with the same distribution of wavelengths.

Atomic model

The constantly accelerating electron in the Hydrogen atom is moving on the equipotential line of the proton and it's kinetic and potential energy will be constant. Its energy will change only when it is changing its way to another equipotential line with another value of potential energy or getting free with enough kinetic energy. This means that the Rutherford-Bohr atomic model is right and only that changing acceleration of the electric charge causes radiation, not the steady acceleration. The steady acceleration of the charges only creates a centric parabolic steady electric field around the charge, the magnetic field. This gives the magnetic moment of the atoms, summing up the proton and electron magnetic moments caused by their circular motions and spins.

The Relativistic Bridge

Commonly accepted idea that the relativistic effect on the particle physics it is the fermions' spin - another unresolved problem in the classical concepts. If the electric charges can move only with accelerated motions in the self maintaining electromagnetic field, once upon a time they would reach the velocity of the electromagnetic field. The resolution of this problem is the spinning particle, constantly accelerating and not reaching the velocity of light because the acceleration is radial. One origin of the Quantum Physics is the Planck Distribution Law of the electromagnetic oscillators, giving equal intensity for 2 different wavelengths on any temperature. Any of these two wavelengths will give equal intensity diffraction patterns, building different asymmetric constructions, for example proton - electron structures (atoms), molecules, etc. Since the particles are centers of diffraction patterns they also have particle – wave duality as the electromagnetic waves have. [2]

The weak interaction

The weak interaction transforms an electric charge in the diffraction pattern from one side to the other side, causing an electric dipole momentum change, which violates the CP and time reversal symmetry. The Electroweak Interaction shows that the Weak Interaction is basically electromagnetic in nature. The arrow of time shows the entropy grows by changing the temperature dependent diffraction patterns of the electromagnetic oscillators.

Another important issue of the quark model is when one quark changes its flavor such that a linear oscillation transforms into plane oscillation or vice versa, changing the charge value with 1 or -1. This kind of change in the oscillation mode requires not only parity change, but also charge and time changes (CPT symmetry) resulting a right handed anti-neutrino or a left handed neutrino.

The right handed anti-neutrino and the left handed neutrino exist only because changing back the quark flavor could happen only in reverse, because they are different geometrical constructions, the u is 2 dimensional and positively charged and the d is 1 dimensional and negatively charged. It needs also a time reversal, because anti particle (anti neutrino) is involved.

The neutrino is a 1/2spin creator particle to make equal the spins of the weak interaction, for example neutron decay to 2 fermions, every particle is fermions with ½ spin. The weak interaction changes the entropy since more or less particles will give more or less freedom of movement. The entropy change is a result of temperature change and breaks the equality of oscillator diffraction intensity of the Maxwell–Boltzmann statistics. This way it changes the time coordinate measure and
makes possible a different time dilation as of the special relativity.

The limit of the velocity of particles as the speed of light appropriate only for electrical charged particles, since the accelerated charges are self maintaining locally the accelerating electric force. The neutrinos are CP symmetry breaking particles compensated by time in the CPT symmetry, that is the time coordinate not works as in the electromagnetic interactions, consequently the speed of neutrinos is not limited by the speed of light.

The weak interaction T-asymmetry is in conjunction with the T-asymmetry of the second law of thermodynamics, meaning that locally lowering entropy (on extremely high temperature) causes the
weak interaction, for example the Hydrogen fusion.

Probably because it is a spin creating movement changing linear oscillation to 2 dimensional oscillation by changing d to u quark and creating anti neutrino going back in time relative to the proton and electron created from the neutron, it seems that the anti neutrino fastest then the velocity of the photons created also in this weak interaction?

A quark flavor changing shows that it is a reflection changes movement and the CP- and T-symmetry breaking!!! This flavor changing oscillation could prove that it could be also on higher level such as atoms, molecules, probably big biological significant molecules and responsible on the aging of the life.

Important to mention that the weak interaction is always contains particles and antiparticles, where the neutrinos (antineutrinos) present the opposite side. It means by Feynman's interpretation that these particles present the backward time and probably because this they seem to move faster than the speed of light in the reference frame of the other side.

Finally since the weak interaction is an electric dipole change with ½ spin creating; it is limited by the velocity of the electromagnetic wave, so the neutrino's velocity cannot exceed the velocity of light.

The General Weak Interaction

The Weak Interactions T-asymmetry is in conjunction with the T-asymmetry of the Second Law of Thermodynamics, meaning that locally lowering entropy (on extremely high temperature) causes for example the Hydrogen fusion. The arrow of time by the Second Law of Thermodynamics shows the increasing entropy and decreasing information by the Weak Interaction, changing the temperature dependent diffraction patterns. A good example of this is the neutron decay, creating more particles with less known information about them.

The neutrino oscillation of the Weak Interaction shows that it is a general electric dipole change and it is possible to any other temperature dependent entropy and information changing diffraction pattern of atoms, molecules and even complicated biological living structures.

We can generalize the weak interaction on all of the decaying matter constructions, even on the biological too. This gives the limited lifetime for the biological constructions also by the arrow of time. There should be a new research space of the Quantum Information Science the 'general neutrino oscillation' for the greater then subatomic matter structures as an electric dipole change. There is also connection between statistical physics and evolutionary biology, since the arrow of time is working in the biological evolution also.

The Fluctuation Theorem says that there is a probability that entropy will flow in a direction opposite to that dictated by the Second Law of Thermodynamics. In this case the Information is growing that is the matter formulas are emerging from the chaos. So the Weak Interaction has two directions, samples for one direction is the Neutron decay, and Hydrogen fusion is the opposite direction.

Fermions and Bosons

The fermions are the diffraction patterns of the bosons such a way that they are both sides of the same thing.

Van Der Waals force

Named after the Dutch scientist Johannes Diderik van der Waals – who first proposed it in 1873 to explain the behaviour of gases – it is a very weak force that only becomes relevant when atoms and molecules are very close together. Fluctuations in the electronic cloud of an atom mean that it will have an instantaneous dipole moment. This can induce a dipole moment in a nearby atom, the result being an attractive dipole–dipole interaction.

Electromagnetic inertia and mass

Electromagnetic Induction

Since the magnetic induction creates a negative electric field as a result of the changing acceleration, it works as an electromagnetic inertia, causing an electromagnetic mass. [1]

Relativistic change of mass

The increasing mass of the electric charges the result of the increasing inductive electric force acting against the accelerating force. The decreasing mass of the decreasing acceleration is the result of the inductive electric force acting against the decreasing force. This is the relativistic mass change explanation, especially importantly explaining the mass reduction in case of velocity decrease.

The frequency dependence of mass

Since $E = h\nu$ and $E = mc^2$, $m = h\nu /c^2$ that is the m depends only on the ν frequency. It means that the mass of the proton and electron are electromagnetic and the result of the electromagnetic induction, caused by the changing acceleration of the spinning and moving charge! It could be that the m_o inertial mass is the result of the spin, since this is the only accelerating motion of the electric charge. Since the accelerating motion has different frequency for the electron in the atom and the proton, they masses are different, also as the wavelengths on both sides of the diffraction pattern, giving equal intensity of radiation.

Electron – Proton mass rate

The Planck distribution law explains the different frequencies of the proton and electron, giving equal intensity to different lambda wavelengths! Also since the particles are diffraction patterns they have some closeness to each other – can be seen as a gravitational force. [2]

There is an asymmetry between the mass of the electric charges, for example proton and electron, can understood by the asymmetrical Planck Distribution Law. This temperature dependent energy distribution is asymmetric around the maximum intensity, where the annihilation of matter and antimatter is a high probability event. The asymmetric sides are creating different frequencies of electromagnetic radiations being in the same intensity level and compensating each other. One of these compensating ratios is the electron – proton mass ratio. The lower energy side has no compensating intensity level, it is the dark energy and the corresponding matter is the dark matter.

Gravity from the point of view of quantum physics

The Gravitational force

The gravitational attractive force is basically a magnetic force.

The same electric charges can attract one another by the magnetic force if they are moving parallel in the same direction. Since the electrically neutral matter is composed of negative and positive charges they need 2 photons to mediate this attractive force, one per charges. The Bing Bang caused parallel moving of the matter gives this magnetic force, experienced as gravitational force.

Since graviton is a tensor field, it has spin = 2, could be 2 photons with spin = 1 together.

You can think about photons as virtual electron – positron pairs, obtaining the necessary virtual mass for gravity.

The mass as seen before a result of the diffraction, for example the proton – electron mass rate $M_p = 1840 \, M_e$. In order to move one of these diffraction maximum (electron or proton) we need to intervene into the diffraction pattern with a force appropriate to the intensity of this diffraction maximum, means its intensity or mass.

The Big Bang caused acceleration created radial currents of the matter, and since the matter is composed of negative and positive charges, these currents are creating magnetic field and attracting forces between the parallel moving electric currents. This is the gravitational force experienced by the matter, and also the mass is result of the electromagnetic forces between the charged particles. The positive and negative charged currents attracts each other or by the magnetic forces or by the much stronger electrostatic forces!?

The gravitational force attracting the matter, causing concentration of the matter in a small space and leaving much space with low matter concentration: dark matter and energy.
There is an asymmetry between the mass of the electric charges, for example proton and electron, can understood by the asymmetrical Planck Distribution Law. This temperature dependent energy distribution is asymmetric around the maximum intensity, where the annihilation of matter and antimatter is a high probability event. The asymmetric sides are creating different frequencies of electromagnetic radiations being in the same intensity level and compensating each other. One of these compensating ratios is the electron – proton mass ratio. The lower energy side has no compensating intensity level, it is the dark energy and the corresponding matter is the dark matter.

The Higgs boson

By March 2013, the particle had been proven to behave, interact and decay in many of the expected ways predicted by the Standard Model, and was also tentatively confirmed to have + parity and zero spin, two fundamental criteria of a Higgs boson, making it also the first known scalar particle to be discovered in nature, although a number of other properties were not fully proven and some partial results do not yet precisely match those expected; in some cases data is also still awaited or being analyzed.

Since the Higgs boson is necessary to the W and Z bosons, the dipole change of the Weak interaction and the change in the magnetic effect caused gravitation must be conducted. The Wien law is also important to explain the Weak interaction, since it describes the T_{max} change and the diffraction patterns change. [2]

Higgs mechanism and Quantum Gravity

The magnetic induction creates a negative electric field, causing an electromagnetic inertia. Probably it is the mysterious Higgs field giving mass to the charged particles? We can think about the photon as an electron-positron pair, they have mass. The neutral particles are built from negative and positive charges, for example the neutron, decaying to proton and electron. The wave – particle duality makes sure that the particles are oscillating and creating magnetic induction as an inertial mass, explaining also the relativistic mass change. Higher frequency creates stronger magnetic induction, smaller frequency results lesser magnetic induction. It seems to me that the magnetic induction is the secret of the Higgs field.

In particle physics, the Higgs mechanism is a kind of mass generation mechanism, a process that gives mass to elementary particles. According to this theory, particles gain mass by interacting with the Higgs field that permeates all space. More precisely, the Higgs mechanism endows gauge bosons in a gauge theory with mass through absorption of Nambu–Goldstone bosons arising in spontaneous symmetry breaking.

The simplest implementation of the mechanism adds an extra Higgs field to the gauge theory. The spontaneous symmetry breaking of the underlying local symmetry triggers conversion of components of this Higgs field to Goldstone bosons which interact with (at least some of) the other fields in the theory, so as to produce mass terms for (at least some of) the gauge bosons. This mechanism may also leave behind elementary scalar (spin-0) particles, known as Higgs bosons.

In the Standard Model, the phrase "Higgs mechanism" refers specifically to the generation of masses for the $W^{\pm}$, and Z weak gauge bosons through electroweak symmetry breaking. The Large Hadron Collider at CERN announced results consistent with the Higgs particle on July 4, 2012 but stressed that further testing is needed to confirm the Standard Model.

What is the Spin?

So we know already that the new particle has spin zero or spin two and we could tell which one if we could detect the polarizations of the photons produced. Unfortunately this is difficult and neither ATLAS nor CMS are able to measure polarizations. The only direct and sure way to confirm that the particle is indeed a scalar is to plot the angular distribution of the photons in the rest frame of the centre of mass. A spin zero particles like the Higgs carries no directional information away from the original collision so the distribution will be even in all directions. This test will be possible when a much larger number of events have been observed. In the mean time we can settle for less certain indirect indicators.

The Graviton

In physics, the graviton is a hypothetical elementary particle that mediates the force of gravitation in the framework of quantum field theory. If it exists, the graviton is expected to be massless (because the gravitational force appears to have unlimited range) and must be a spin-2 boson. The spin follows from the fact that the source of gravitation is the stress-energy tensor, a second-rank tensor (compared to electromagnetism's spin-1 photon, the source of which is the four-current, a first-rank tensor). Additionally, it can be shown that any massless spin-2 field would give rise to a force indistinguishable from gravitation, because a massless spin-2 field must couple to (interact with) the stress-energy tensor in the same way that the gravitational field does. This result suggests

that, if a massless spin-2 particle is discovered, it must be the graviton, so that the only experimental verification needed for the graviton may simply be the discovery of a massless spin-2 particle. [3]

The Secret of Quantum Entanglement

The Secret of Quantum Entanglement that the particles are diffraction patterns of the electromagnetic waves and this way their quantum states every time is the result of the quantum state of the intermediate electromagnetic waves. [2] When one of the entangled particles wave function is collapses by measurement, the intermediate photon also collapses and transforms its state to the second entangled particle giving it the continuity of this entanglement. Since the accelerated charges are self-maintaining their potential locally causing their acceleration, it seems that they entanglement is a spooky action at a distance.

Conclusions

The accelerated charges self-maintaining potential shows the locality of the relativity, working on the quantum level also.
The Secret of Quantum Entanglement that the particles are diffraction patterns of the electromagnetic waves and this way their quantum states every time is the result of the quantum state of the intermediate electromagnetic waves.
One of the most important conclusions is that the electric charges are moving in an accelerated way and even if their velocity is constant, they have an intrinsic acceleration anyway, the so called spin, since they need at least an intrinsic acceleration to make possible they movement .
The bridge between the classical and quantum theory is based on this intrinsic acceleration of the spin, explaining also the Heisenberg Uncertainty Principle. The particle – wave duality of the electric charges and the photon makes certain that they are both sides of the same thing. Basing the gravitational force on the accelerating Universe caused magnetic force and the Planck Distribution Law of the electromagnetic waves caused diffraction gives us the basis to build a Unified Theory of the physical interactions.

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