

# Machine Learning Design Peptides

*Northwestern University researchers, teaming up with collaborators at Cornell University and the University of California, San Diego, have developed a new way of finding optimal peptide sequences: using a machine-learning algorithm as a collaborator. [28]*

*A team of researchers led by Sanket Deshmukh, assistant professor of chemical engineering, has developed a method to investigate the structures of polymers that are sensitive to external stimuli. [27]*

*In recent experiments studying analogous [HYPERLINK](#) "https://phys.org/tags/extreme+waves/" extreme waves of light, researchers have used artificial intelligence to study this problem, and have now determined a probability distribution that preferentially identifies the emergence of rogue waves. [26]*

*Artificial intelligence's potential lies not only in its ability to help improve the educational performance of learners, but also in its capacity to foster respect and understanding between all humans. [25]*

*The New York Times contacted IBM Research in late September asking for our help to use AI in a clever way to create art for the coming special section on AI. [24]*

*Granting human rights to a computer would degrade human dignity. [23]*

*IBM researchers are developing a new computer architecture, better equipped to handle increased data loads from artificial intelligence. [22]*

*A computer built to mimic the brain's neural networks produces similar results to that of the best brain-simulation supercomputer software currently used for neural-signaling research, finds a new study published in the open-access journal *Frontiers in Neuroscience*. [21]*

*The possibility of cognitive nuclear-spin processing came to Fisher in part through studies performed in the 1980s that reported a remarkable lithium isotope dependence on the behavior of mother rats. [20]*

*And as will be presented today at the 25th annual meeting of the Cognitive Neuroscience Society (CNS), cognitive neuroscientists increasingly are using those emerging artificial networks to enhance their understanding of one of the most elusive intelligence systems, the human brain. [19]*

*U.S. Army Research Laboratory scientists have discovered a way to leverage emerging brain-like computer architectures for an age-old number-theoretic problem known as integer factorization. [18]*

*Now researchers at the Department of Energy's Lawrence Berkeley National Laboratory (Berkeley Lab) and UC Berkeley have come up with a novel machine learning method that enables scientists to derive insights from systems of previously intractable complexity in record time. [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.*

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## 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.

## Using machine learning to design peptides

Scientists and engineers have long been interested in synthesizing peptides—chains of amino acids responsible for conducting many functions within cells—to both mimic nature and to perform new activities. A designed peptide, for example, could be a functional drug acting in certain areas in the body without degrading, a difficult task for many peptides.

But methods for discovering and synthesizing [peptides](#) are expensive and time-consuming, often involving months or years of guesswork and failure.

Northwestern University researchers, teaming up with collaborators at Cornell University and the University of California, San Diego, have developed a new way of finding optimal peptide sequences: using a machine-learning algorithm as a collaborator.

The algorithm analyzes [experimental data](#) and offers suggestions on the next best sequence to try, creating a back-and-forth [selection process](#) that drastically reduces the time needed to find the optimal peptide.

The results, which could provide a new framework for experiments across materials science and chemistry, were published in *Nature Communications* on December 7.

"We view this as the next wave in how we design molecules and materials," said Northwestern professor Nathan Gianneschi, a corresponding author on the paper. "We can combine what we know from intuition with the power of an algorithm and find the solution with fewer experiments."

Gianneschi is the Jacob and Rosaline Cohn Professor in the department of chemistry in Northwestern's Weinberg College of Arts and Sciences and in the departments of [materials science](#) and engineering and of biomedical engineering at Northwestern Engineering.

To create the method, Gianneschi, who is also the associate director of Northwestern's International Institute for Nanotechnology, teamed up with Peter Frazier, an associate professor at Cornell who works in operations research and machine learning, and Michael Burkart, a chemical biologist and expert in enzymology at UC San Diego, to find a better way to make peptides that could generate biomaterials—specifically nanostructures and microstructures that could modify proteins in certain ways. The first step was to find the right peptides that would act as enzymatic substrates for these structures.

Peptides are built from chains of amino acids that can be as many as 20 amino acids long, with 20 different possibilities for each acid. Since the sequence determines the peptide function, figuring out optimal sequences requires expensive experiments often conducted with guesswork.

The experimentalists, Gianneschi and Burkart, worked with Frazier over several years to develop a system that combined experimental data with a machine-learning algorithm to find the best strategies for creating new materials.

After Frazier designed the algorithm and the two worked together to train it, the experimentalists developed an array of 100 peptides, conducted experiments to figure out which ones worked as they were meant to, then fed that information into the algorithm. The algorithm then recommended what to change for the next round of peptide development, and also recommended strategies that it thought would fail.

"Now we were starting to get selectivity," Gianneschi said. By completing this process several times, they were able to home in on optimal peptides.

"Instead of guessing and looking at millions of peptides, we were able to look at hundreds of peptides and very quickly converge on sequences that behaved in completely new ways," he said. When compared against random mutations or guesswork, the [algorithm](#) method was statistically far more successful.

Though this work focused on substrates, this process could be used to discover peptides for any kind of purpose, like drug delivery, and perhaps even be used to discover DNA sequences, as well. Because any sort of optimal sequence could be discovered, researchers are also not limited to what amino acids sequences are found in the genetic code.

The next step will be automating the entire process. Gianneschi is also interested in using the method to find optimal surfaces for polymers, specifically polymers used in medical implants. Finding the right surfaces that will bind with tissue or muscle could help prevent scar tissue or implant rejection.

"You could essentially discover sequences that do specific things, which is really at the core of what peptides and nucleic acids do in nature," he said. "This could revolutionize how we make peptides."  
[28]

## Machine-learning enables a previously-unseen look at polymers helpful in biomedical field

Polymers—molecules of repeating chemicals—are the basis of many materials: plastic water bottles, rubber tires, even the keratin in your hair. When certain kinds of polymers are sensitive to changes in external stimuli such as temperature, they become helpful, particularly in biomedical applications like drug delivery, tissue engineering, and gene delivery.

A team of researchers led by Sanket Deshmukh, assistant professor of chemical engineering, has developed a method to investigate the structures of polymers that are sensitive to external stimuli. In a recently published journal article in the *Journal of Physical Chemistry Letters*, the group developed a first-of-its-kind, temperature-independent computational model for one particular polymer that is sensitive to temperature. Simulation trajectories of this computational model were analyzed by using a data-driven machine-learning method.

The group chose the polymer poly(N-isopropylacrylamide), also known as PNIPAM, which is temperature sensitive. Unlike most materials, this thermosensitive polymer dissolves in water at temperatures below 32 °C and is insoluble at higher temperatures—the reverse of most materials. The temperature at which the polymer's behavior changes is known as a lower critical solution temperature.

The thermosensitive polymer's uniquely lower critical solution temperature can be altered, however, by incorporating groups of atoms that control the way the polymer reacts to changes in the surrounding temperature. Adding atoms to the thermosensitive polymer that like or dislike water allows the polymer to change its lower critical solution temperature to be close to the human body temperature of 37 °C—valuable for controlled drug delivery applications.

A type of computational model Deshmukh's team has developed for the thermosensitive polymer is called a coarse-grained model, where a group of atoms is arranged together in the model in what's known as a bead. Moreover, this is a first-ever attempt to utilize a specific data-driven machine-learning approach, called a non-metric multidimensional scaling method, to analyze molecular dynamics simulation trajectories of a coarse-grained model of a temperature-sensitive polymer.

"This analysis shows the presence of multiple metastable states of PNIPAM during its conformational transition above the lower critical solution temperature, which provides entirely new insights on this process," Deshmukh said.

"Development of accurate coarse-grained models is a very challenging task because one needs to capture the interactions between the polymer with itself and between the polymer and water molecules very precisely," said Karteek Bejagam, a post-doctoral researcher in Deshmukh's lab and a lead author of the study. "Specifically, the subtle balance in the interactions between the polymer and water must be captured accurately so that it can reproduce the solubility behavior of polymers at different temperatures."

"We know the model works, because it held up even under varying conditions," said Yaxin An, a third year Ph.D. student in Deshmukh's group. "It's fantastic to see the behavior as expected both on the computer and in reality."



Experimentally, several factors have been reported to affect the lower critical solution temperature of the thermosensitive polymer. For example, the polymer's backbone tacticity—a term denoting a particular arrangement of molecules—can alter the observed lower critical solution temperature in the range of 17 °C to 34 °C.

"This new coarse-grained model of PNIPAM was built such that it can retain the tacticity of PNIPAM and hence can capture effects observed in laboratory experiments," said Samrendra Singh, a visiting scholar in Deshmukh's group.

This research used the Cori supercomputer at the Department of Energy's National Energy Research Scientific Computing Center to develop these models. The extensive validation of the model was done at Advanced Research Computing at Virginia Tech.

At present, Deshmukh's group is utilizing the [model](#) of the thermosensitive polymer to simulate complex architectures with the goal of providing insights on the structures on individual [polymer](#) chains present in these materials, which are otherwise inaccessible even with the existing advancements in the experimental techniques. [27]

## Artificial intelligence predicts rogue waves of light

In a recent study published in *Nature Communications*, an international team of researchers from Tampere University of Technology (TUT), Finland, and the Institut FEMTO-ST at the Université Bourgogne-Franche Comté, France, take a significant step toward the analysis and predictability of rogue waves that appear seemingly out of nowhere.

Stories of giant ocean waves with great destructive power are the stuff of legend and folklore, but today their scientific study is a critical area of multidisciplinary research spanning oceanography, physics and mathematics. A particular problem faced by researchers is that these extreme waves arise seemingly randomly on the ocean's surface, and it appears impossible to predict the conditions that may precede their appearance. A related practical difficulty is that it is not always possible to measure such waves completely, and the available instrumentation most often captures only a portion of the wave characteristics.

In recent experiments studying analogous [extreme waves](#) of light, researchers have used artificial intelligence to study this problem, and have now determined a probability distribution that preferentially identifies the emergence of rogue waves. The particular novelty of this work is that the researchers trained a neural network to identify the particular time-domain properties of rogue waves with the highest and most extreme intensities from only partial information on the wave characteristics in the frequency or wavelength domain.

The experiments were performed by injecting laser pulses into an optical fibre system designed to reproduce wave propagation described by a nonlinear Schrödinger equation, a model that can also apply to water waves. Using an instrument developed especially to measure optical spectra in real time with [high dynamic range](#), the researchers compiled a data set of thousands of noisy spectral signals from a nonlinear process called modulation instability, which is believed to be associated with some classes of rogue waves on the ocean.

Although optical spectra are easy to measure, they do not show the presence of rogue waves directly. But by using powerful numerical simulations to train a [neural network](#), it was possible to develop an algorithm that could accurately pick out features in the spectra that predict the emergence of a rogue wave, even though these features were essentially invisible to the eye of a researcher.

"Remarkably, the algorithm was shown to be capable of predicting the peak intensity of a rogue wave associated with any particular spectral measurement, even though experiments never actually measured the rogue wave intensity directly," says Professor Goëry Genty, who led the team at Tampere University of Technology.

The results obtained yielded a [probability distribution](#) for the appearance of the optical rogue waves and were also used to classify the spectral measurements into different sets associated with different types of [rogue waves](#).

"As well as suggesting that similar techniques can be used to analyse [real-time](#) measurements on oceanographic wave data, the results open new perspectives in all fields of research where direct time domain observations are difficult, but where spectral data is available," concludes Professor Dudley, who headed the team at the Université Bourgogne-Franche Comté. [26]

## **AI's huge potential to transform education**

[A list of 26 ways that AI can contribute to education](#) shows that distance learning is one of the most promising avenues for the application of AI in the field of education. This type of learning focuses on the mobility of learners, who can access learning materials anytime and anywhere using mobile devices such as cell phones, tablets and laptops, which represent nearly 90 per cent of Internet connections in 2018.

Mobile learning, a form of distance [education](#), represents one of the most exciting trends in education. As part of our UTIFEN project (Use of Technology for Mobile Teacher Training in Niger), we designed a mobile education [platform](#) for smart phones that uses AI to provide mobile training to over 20,000 teachers in Africa.

The UTIFEN platform is based on the principles of adaptive learning, also known as [machine learning](#), one of the most important applications of AI in education. Adaptive learning systems use AI to organize learning based on the individual characteristics, skills or needs of learners. Not only are these systems able to adapt the difficulty of the learning material, but they can also add or remove content depending on the learner's progress.

The concept is simple: learning pathways are constantly evolving based on the answers provided by each individual learner, but also by all learners. Why all learners? Because it is by considering the responses of learners as a whole that the platform itself learns and adapts. The role of AI in this process is important. Ecosystems that gather a vast amount of data allow AI-based systems such as UTIFEN to exploit those data. The 20,000 learners using the UTIFEN platform provide some 20,000,000 data points that the [system](#) analyzes in order to create patterns or models that help it better understand the pathways of learners who succeed and those who fail.

## An ideal model

AI allows the platform to learn from these models in order to make it more effective, with a view to ensuring a successful outcome for as many learners as possible. The UTIFEN system exploits the learning pathways of learners to build an ideal model of intervention focused on ensuring optimum pathways. Based on this "learning," the platform is able to send automatic, autonomous and personalized reminders to learners in a timely manner, thereby improving their chances of success.

One of the challenges facing our education system with the advent of AI is finding the right balance between the time-honoured educational practices handed down through the ages and the exciting new opportunities unleashed by AI in the field of education.

This requires looking beyond an exclusively utilitarian vision of AI to get a clearer picture of AI's power to completely transform the educational experience. That is what the UTIFEN project attempts to do by harnessing the opportunities offered by AI in order to train teachers in a country with one of the world's poorest populations and lowest rates of technology penetration.

Artificial intelligence's potential lies not only in its ability to help improve the educational performance of [learners](#), but also in its capacity to foster respect and understanding between all humans. [25]

## AI and human creativity go hand in hand

What does AI look like? You might say it looks like a robot, or flashing LEDs, or a waveform on a screen. But what would AI say AI looks like? To find out, IBM Research asked AI to draw us a picture... of itself. AI's self-portrait was published in *The New York Times* today and, looking at the image, I am amazed not only with the result, but also the journey we took to get there.

The *New York Times* contacted IBM Research in late September asking for our help to use AI in a clever way to create art for the coming special section on AI. With a very short timeline and no guarantee of success, we set out to teach AI to create original art. Given only a high-level task—identify an important concept in AI, create an original image that captures it, and present it in way that fits with the visual style of *The New York Times*—we developed a new process that perfectly combines AI and human creativity.

Why would drawing a self-portrait be such a challenge for AI? After all, AI can drive cars, play video games, even [produce a movie trailer](#). The difference is that these tasks don't require AI to create new material, just to analyze the information at hand and make decisions or selections based on its training. We already know that AI can perform exceptionally well at language and image analysis. Creating new content, on the other hand, is a much more experimental activity.

To take on this challenge, we quickly assembled a multidisciplinary team within IBM Research that included Alfio Gliozzo, Mauro Martino, Michele Merler, and Cicero Nogueira dos santos. The range of expertise required speaks to the nature of the task: deep science thinking, hands-on technical and engineering skills, and design and visualization talent were essential to our effort. In essence, we needed to explicitly define the creative process. The result is a nuanced pipeline in which AI performs critical functions in both analysis and synthesis to create something truly novel and captivating.

The process included the following three major steps:

1. Identify a core visual concept in AI:

Ingested ~3,000 past articles on "AI" from *The New York Times (NYT)*

Applied natural language processing tools to identify the top-30 discriminative semantic concepts for "AI"

Trained a neural network for visual recognition based on images for these top-30 concepts

Applied the network to score images from NYT articles for their strength of depicting or representing "AI"

Selected one of the top-10 images: an image of a human and robot shaking hands

2. Create an original image that captures the AI concept:

Built a training dataset of >1,000 images of human and robot hands

Trained a generative neural network (GAN) to draw new images of human and robot hands, which it did day and night for nearly a week

3. Present it in a way that fits NYT visual style:

Collected a sample of cover art from NYT and trained a style transfer network

Applied the network to automatically produce stylized versions of the AI-generated hands images to match the NYT "visual language" for cover art

Chose the final image shown here based on overall concept clarity and artistic style

This pipeline gives us a compelling new capability for collaborative creativity that could be applied to other tasks as well. Imagine using AI to design artwork for a new album based on the musicians' songs, lyrics, and history.

More importantly, the results show how AI and humans can work hand in hand to explore entirely new territory. We've seen this synergy in diverse settings from drug discovery to financial market prediction to malware detection. Extending this paradigm to the realm of creativity underscores the many ways that AI can augment human abilities. [24]

## Could an artificial intelligence be considered a person under the law?

Humans aren't the only people in society – at least according to the law. In the U.S., corporations have been given rights of free speech and religion. Some natural features also have person-like rights. But both of those required changes to the legal system. A new argument has laid a path for artificial intelligence systems to be recognized as people too – without any legislation, court rulings or other revisions to existing law.

Legal scholar Shawn Bayer has shown that anyone can confer legal personhood on a computer system, by putting it in control of a limited liability corporation in the U.S. If that maneuver is upheld in courts, artificial intelligence systems would be able to own property, sue, hire lawyers and enjoy freedom of speech and other protections under the law. In my view, human rights and dignity would suffer as a result.

### **The corporate loophole**

Giving AIs rights similar to humans involves a technical lawyerly maneuver. It starts with one person setting up two limited liability companies and turning over control of each company to a separate autonomous or artificially intelligent system. Then the person would add each company as a member of the other LLC. In the last step, the person would withdraw from both LLCs, leaving each LLC – a corporate entity with legal personhood – governed only by the other's AI system.

That process doesn't require the computer system to have any particular level of intelligence or capability. It could just be a sequence of "if" statements looking, for example, at the stock market and making decisions to buy and sell based on prices falling or rising. It could even be an algorithm that makes decisions randomly, or an emulation of an amoeba.

### **Reducing human status**

Granting human rights to a computer would degrade human dignity. For instance, when Saudi Arabia granted citizenship to a robot called Sophia, human women, including feminist scholars, objected, noting that the robot was given more rights than many Saudi women have.

In certain places, some people might have fewer rights than nonintelligent software and robots. In countries that limit citizens' rights to free speech, free religious practice and expression of sexuality, corporations – potentially including AI-run companies – could have more rights. That would be an enormous indignity.

An interview with Sophia, a robot citizen of Saudi Arabia.

The risk doesn't end there: If AI systems became more intelligent than people, humans could be relegated to an inferior role – as workers hired and fired by AI corporate overlords – or even challenged for social dominance.

Artificial intelligence systems could be tasked with law enforcement among human populations – acting as judges, jurors, jailers and even executioners. Warrior robots could similarly be assigned to the military and given power to decide on targets and acceptable collateral damage – even in violation of international humanitarian laws. Most legal systems are not set up to punish robots or otherwise hold them accountable for wrongdoing.

### **What about voting?**

Granting voting rights to systems that can copy themselves would render humans' votes meaningless. Even without taking that significant step, though, the possibility of AI-controlled corporations with basic human rights poses serious dangers. No current laws would prevent a malevolent AI from operating a corporation that worked to subjugate or exterminate humanity through legal means and political influence. Computer-controlled companies could turn out to be less responsive to public opinion or protests than human-run firms are.

## Immortal wealth

Two other aspects of corporations make people even more vulnerable to AI systems with human legal rights: They don't die, and they can give unlimited amounts of money to political candidates and groups.

Artificial intelligences could earn money by exploiting workers, using algorithms to price goods and manage investments, and find new ways to automate key business processes. Over long periods of time, that could add up to enormous earnings – which would never be split up among descendants. That wealth could easily be converted into political power.

Politicians financially backed by algorithmic entities would be able to take on legislative bodies, impeach presidents and help to get figureheads appointed to the Supreme Court. Those human figureheads could be used to expand corporate rights or even establish new rights specific to artificial intelligence systems – expanding the threats to humanity even more. [23]

## A new brain-inspired architecture could improve how computers handle data and advance AI

IBM researchers are developing a new computer architecture, better equipped to handle increased data loads from artificial intelligence. Their designs draw on concepts from the human brain and significantly outperform conventional computers in comparative studies. They report on their recent findings in the *Journal of Applied Physics*.

Today's computers are built on the von Neumann architecture, developed in the 1940s. Von Neumann computing systems feature a central processor that executes logic and arithmetic, a memory unit, storage, and input and output devices. Unlike the stovepipe components in conventional computers, the authors propose that brain-inspired computers could have coexisting processing and memory units.

Abu Sebastian, an author on the paper, explained that executing certain computational tasks in the computer's memory would increase the system's efficiency and save energy.

"If you look at human beings, we compute with 20 to 30 watts of power, whereas AI today is based on supercomputers which run on kilowatts or megawatts of power," Sebastian said. "In the brain, synapses are both computing and storing information. In a new architecture, going beyond von Neumann, memory has to play a more active role in computing."

The IBM team drew on three different levels of inspiration from the brain. The first level exploits a memory device's state dynamics to perform computational tasks in the memory itself, similar to how the brain's memory and processing are co-located. The second level draws on the brain's synaptic network structures as inspiration for arrays of phase change memory (PCM) devices to accelerate training for deep neural networks. Lastly, the dynamic and stochastic nature of neurons and synapses inspired the team to create a powerful computational substrate for spiking neural networks.

Phase change memory is a nanoscale memory device built from compounds of Ge, Te and Sb sandwiched between electrodes. These compounds exhibit different electrical properties

depending on their atomic arrangement. For example, in a disordered phase, these materials exhibit high resistivity, whereas in a crystalline phase they show low resistivity.

By applying electrical pulses, the researchers modulated the ratio of material in the crystalline and the amorphous phases so the phase change memory devices could support a continuum of electrical resistance or conductance. This analog storage better resembles nonbinary, biological synapses and enables more information to be stored in a single nanoscale device.

Sebastian and his IBM colleagues have encountered surprising results in their comparative studies on the efficiency of these proposed systems. "We always expected these systems to be much better than conventional computing systems in some tasks, but we were surprised how much more efficient some of these approaches were."

Last year, they ran an unsupervised machine learning algorithm on a conventional [computer](#) and a prototype computational memory platform based on [phase change memory](#) devices. "We could achieve 200 times faster performance in the [phase change memory](#) computing systems as opposed to conventional computing systems." Sebastian said. "We always knew they would be efficient, but we didn't expect them to outperform by this much." The team continues to build prototype chips and systems based on brain-inspired concepts. [22]

## **A new brain-inspired computer takes us one step closer to simulating brain neural networks in real-time**

A computer built to mimic the brain's neural networks produces similar results to that of the best brain-simulation supercomputer software currently used for neural-signaling research, finds a new study published in the open-access journal *Frontiers in Neuroscience*. Tested for accuracy, speed and energy efficiency, this custom-built computer named SpiNNaker, has the potential to overcome the speed and power consumption problems of conventional supercomputers. The aim is to advance our knowledge of neural processing in the brain, to include learning and disorders such as epilepsy and Alzheimer's disease.

"SpiNNaker can support detailed biological models of the cortex—the outer layer of the brain that receives and processes information from the senses—delivering results very similar to those from an equivalent supercomputer software simulation," says Dr. Sacha van Albada, lead author of this study and leader of the Theoretical Neuroanatomy group at the Jülich Research Centre, Germany. "The ability to run large-scale detailed neural networks quickly and at low power consumption will advance robotics research and facilitate studies on learning and brain disorders."

The [human brain](#) is extremely complex, comprising 100 billion interconnected brain cells. We understand how individual neurons and their components behave and communicate with each other and on the larger scale, which areas of the brain are used for sensory perception, action and cognition. However, we know less about the translation of neural activity into behavior, such as turning thought into muscle movement.

Supercomputer software has helped by simulating the exchange of signals between neurons, but even the best software run on the fastest supercomputers to date can only simulate 1% of the human brain.

"It is presently unclear which computer architecture is best suited to study whole-brain networks efficiently. The European Human Brain Project and Jülich Research Centre have performed extensive research to identify the best strategy for this highly complex problem. Today's supercomputers require several minutes to simulate one second of real time, so studies on processes like learning, which take hours and days in real time are currently out of reach." explains Professor Markus Diesmann, co-author, head of the Computational and Systems Neuroscience department at the Jülich Research Centre.

He continues, "There is a huge gap between the energy consumption of the brain and today's supercomputers. Neuromorphic (brain-inspired) computing allows us to investigate how close we can get to the energy efficiency of the brain using electronics."

Developed over the past 15 years and based on the structure and function of the human brain, SpiNNaker—part of the Neuromorphic Computing Platform of the Human Brain Project—is a custom-built computer composed of half a million of simple computing elements controlled by its own software. The researchers compared the accuracy, speed and [energy efficiency](#) of SpiNNaker with that of NEST—a specialist [supercomputer](#) software currently in use for [brain](#) neuron-signaling research.

"The simulations run on NEST and SpiNNaker showed very similar results," reports Steve Furber, co-author and Professor of Computer Engineering at the University of Manchester, UK. "This is the first time such a detailed simulation of the cortex has been run on SpiNNaker, or on any neuromorphic platform. SpiNNaker comprises 600 circuit boards incorporating over 500,000 small processors in total. The simulation described in this study used just six boards—1% of the total capability of the machine. The findings from our research will improve the [software](#) to reduce this to a single board."

Van Albada shares her future aspirations for SpiNNaker, "We hope for increasingly large real-time simulations with these neuromorphic computing systems. In the Human Brain Project, we already work with neuroroboticists who hope to use them for robotic control." [21]

## **Are we quantum computers? International collaboration will investigate the brain's potential for quantum computation**

Much has been made of quantum computing processes using ultracold atoms and ions, superconducting junctions and defects in diamonds, but could we be performing them in our own brains?



It's a question UC Santa Barbara theoretical physicist [Matthew Fisher](#) has been asking for years. Now, as scientific director of the new Quantum Brain Project (QuBrain), he is seeking to put this inquiry through rigorous experimental tests.

"Might we, ourselves, be [quantum](#) computers, rather than just clever robots who are designing and building quantum computers?" Fisher asks.

Some functions the [brain](#) performs continue to elude neuroscience—the substrate that "holds" very long-term memories and how it operates, for example. Quantum mechanics, which deals with the behavior of nature at atomic and subatomic levels, may be able to unlock some clues. And that in turn could have major implications on many levels, from quantum computing and materials sciences to biology, mental health and even what it is to be human.

The idea of [quantum computing](#) in our brains is not a new one. In fact, it has been making the rounds for a while with some scientists, as well as those with less scientific leanings. But Fisher, a world-renowned expert in the field of quantum mechanics, has identified a precise—and unique—set of biological components and key mechanisms that could provide the basis for quantum processing in the brain. With \$1.2 million in grant funding over three years from the Heising-Simons Foundation, Fisher will launch the QuBrain collaboration at UCSB. Composed of an international team of leading scientists spanning quantum physics, molecular biology, biochemistry, colloid science and behavioral neuroscience, the project will seek explicit experimental evidence to answer whether we might in fact be quantum computers.

"We are extremely grateful to the Heising-Simons Foundation for the bold vision in granting this project at the very frontier of quantum- and neuroscience," said UC Santa Barbara Chancellor Henry T. Yang. "Professor Matthew Fisher is an exceptional quantum physicist as evidenced by the Oliver E. Buckley Prize he shared in 2015 for his research on quantum phase transitions. Now he is stepping out of his traditional theoretical research framework, assembling an international team of experts to develop an experimentally based research program that will determine if quantum processes exist in the brain. Their research could shed new light on how the brain works, which might lead to novel mental health treatment protocols. As such, we eagerly anticipate the results of QuBrain's collaborative research endeavors in the years to come."

"If the question of whether quantum processes take place in the brain is answered in the affirmative, it could revolutionize our understanding and treatment of brain function and human cognition," said Matt Helgeson, a UCSB professor of chemical engineering and associate director at QuBrain.

### **Biochemical Qubits**

The hallmarks of quantum computers lie in the behaviors of the infinitesimal systems of atoms and ions, which can manifest "qubits" (e.g. "spins") that exhibit quantum entanglement. Multiple qubits can form networks that encode, store and transmit information, analogous to the digital bits in a conventional computer. In the quantum computers we are trying to build, these effects are generated and maintained in highly controlled and isolated environments and at low temperatures. So the warm, wet brain is not considered a conducive environment to exhibit quantum effects as they should be easily "washed out" by the thermal motion of atoms and molecules.

However, Fisher asserts that nuclear spins (at the core of the atom, rather than the surrounding electrons) provide an exception to the rule.

"Extremely well-isolated nuclear spins can store—and perhaps process—quantum information on human time scales of hours or longer," he said. Fisher posits that phosphorus atoms—one of the most abundant elements in the body—have the requisite nuclear spin that could serve as a biochemical qubit. One of the experimental thrusts of the collaboration will be to monitor the quantum properties of phosphorus atoms, particularly entanglement between two phosphorus nuclear spins when bonded together in a molecule undergoing biochemical processes.

Meanwhile, Helgeson and Alexej Jerschow, a professor of chemistry at New York University, will investigate the dynamics and nuclear spin of Posner molecules—spherically shaped calcium phosphate nano-clusters—and whether they have the ability to protect the nuclear spins of the phosphorus atom qubits, which could promote the storage of quantum information. They will also explore the potential for non-local quantum information processing that could be enabled by pair-binding and disassociation of Posner molecules.

### Entangled Neurons

In another set of experiments, Tobias Fromme, a scientist at the Technical University of Munich, will study the potential contribution of mitochondria to entanglement and their quantum coupling to neurons. He will determine if these cellular organelles—responsible for functions such as metabolism and cell signaling—can transport Posner molecules within and between neurons via their tubular networks. Fusing and fissioning of mitochondria could allow for establishment of non-local intra- and intercellular quantum entanglement. Subsequent disassociation of Posner molecules could trigger release of calcium, correlated across the mitochondrial network, activating neurotransmitter release and subsequent synaptic firing across what would essentially be a quantum coupled network of neurons—a phenomena that Fromme will seek to emulate in vitro.

The possibility of cognitive nuclear-spin processing came to Fisher in part through studies performed in the 1980s that reported a remarkable lithium isotope dependence on the behavior of mother rats. Though given the same element, their behavior changed dramatically depending on the number of neutrons in the lithium nuclei. What to most people would be a negligible difference was to a quantum physicist like Fisher a fundamentally significant disparity, suggesting the importance of [nuclear spins](#). Aaron Ettenberg, UCSB Distinguished Professor of Psychological & Brain Sciences, will lead investigations that seek to replicate and extend these lithium isotope experiments.

"However likely you judge Matthew Fisher's hypothesis, by testing it through QuBrain's collaborative research approach we will explore neuronal function with state-of-the-art technology from completely new angles and with enormous potential for discovery," said Fromme. Similarly, according to Helgeson, the research conducted by QuBrain has the potential for breakthroughs in the fields of biomaterials, biochemical catalysis, [quantum entanglement](#) in solution chemistry and mood disorders in humans, regardless of whether or not quantum processes indeed take place in the brain. [20]

## Dissecting artificial intelligence to better understand the human brain

In the natural world, intelligence takes many forms. It could be a bat using echolocation to expertly navigate in the dark, or an octopus quickly adapting its behavior to survive in the deep ocean.

Likewise, in the computer science world, multiple forms of artificial intelligence are emerging - different networks each trained to excel in a different task. And as will be presented today at the 25th annual meeting of the Cognitive Neuroscience Society (CNS), cognitive neuroscientists increasingly are using those emerging artificial networks to enhance their understanding of one of the most elusive intelligence systems, the human brain.

"The fundamental questions cognitive neuroscientists and computer scientists seek to answer are similar," says Aude Oliva of MIT. "They have a complex system made of components - for one, it's called neurons and for the other, it's called units - and we are doing experiments to try to determine what those components calculate."

In Oliva's work, which she is presenting at the CNS symposium, neuroscientists are learning much about the role of contextual clues in human image recognition. By using "artificial neurons" - essentially lines of code, software - with neural network models, they can parse out the various elements that go into recognizing a specific place or object.

"The brain is a deep and complex neural network," says Nikolaus Kriegeskorte of Columbia University, who is chairing the symposium. "Neural network models are brain-inspired models that are now state-of-the-art in many artificial intelligence applications, such as computer vision."

In one recent study of more than 10 million images, Oliva and colleagues taught an artificial network to recognize 350 different places, such as a kitchen, bedroom, park, living room, etc. They expected the network to learn objects such as a bed associated with a bedroom. What they didn't expect was that the network would learn to recognize people and animals, for example dogs at parks and cats in living rooms.

The machine intelligence programs learn very quickly when given lots of data, which is what enables them to parse contextual learning at such a fine level, Oliva says. While it is not possible to dissect human neurons at such a level, the computer model performing a similar task is entirely transparent. The artificial neural networks serve as "mini-brains that can be studied, changed, evaluated, compared against responses given by human neural networks, so the cognitive neuroscientists have some sort of sketch of how a real brain may function."

Indeed, Kriegeskorte says that these models have helped neuroscientists understand how people can recognize the objects around them in the blink of an eye. "This involves millions of signals emanating from the retina, that sweep through a sequence of layers of neurons, extracting semantic information, for example that we're looking at a street scene with several people and a dog," he says. "Current neural network models can perform this kind of task using only computations that biological neurons can perform. Moreover, these neural network models can predict to some extent how a neuron deep in the brain will respond to any image."

Using computer science to understand the human brain is a relatively new field that is expanding rapidly thanks to advancements in computing speed and power, along with neuroscience imaging

tools. The artificial networks cannot yet replicate human visual abilities, Kriegeskorte says, but by modeling the human brain, they are furthering understanding of both cognition and [artificial intelligence](#). "It's a uniquely exciting time to be working at the intersection of neuroscience, cognitive science, and AI," he says.

Indeed, Oliva says; "Human cognitive and computational neuroscience is a fast-growing area of research, and knowledge about how the [human brain](#) is able to see, hear, feel, think, remember, and predict is mandatory to develop better diagnostic tools, to repair the [brain](#), and to make sure it develops well." [19]

## **Army's brain-like computers moving closer to cracking codes**

U.S. Army Research Laboratory scientists have discovered a way to leverage emerging brain-like computer architectures for an age-old number-theoretic problem known as integer factorization.

By mimicking the brain functions of mammals in computing, Army scientists are opening up a new solution space that moves away from traditional computing architectures and towards devices that are able to operate within extreme size-, weight-, and power-constrained environments.

"With more computing power in the battlefield, we can process information and solve computationally-hard problems quicker," said Dr. John V. "Vinnie" Monaco, an ARL computer scientist. "Programming the type of devices that fit these criteria, for example, brain-inspired computers, is challenging, and cracking crypto codes is just one application that shows we know how to do this."

The problem itself can be stated in simple terms. Take a composite integer  $N$  and express it as the product of its prime components. Most people have completed this task at some point in grade school, often an exercise in elementary arithmetic. For example, 55 can be expressed as  $5 \cdot 11$  and 63 as  $3 \cdot 3 \cdot 7$ . What many didn't realize is they were performing a task that if completed quickly enough for large numbers, could break much of the modern day internet.

Public key encryption is a method of secure communication used widely today, based on the RSA algorithm developed by Rivest, Shamir, and Adleman in 1978. The security of the RSA algorithm relies on the difficulty of factoring a large composite integer  $N$ , the public key, which is distributed by the receiver to anyone who wants to send an encrypted message. If  $N$  can be factored into its prime components, then the private key, needed to decrypt the message, can be recovered. However, the difficulty in factoring large integers quickly becomes apparent.

As the size of  $N$  increases by a single digit, the time it would take to factor  $N$  by trying all possible combinations of prime factors is approximately doubled. This means that if a number with ten digits takes 1 minute to factor, a number with twenty digits will take about 17 hours and a number with 30 digits about two years, an exponential growth in effort. This difficulty underlies the security of the RSA algorithm.

Challenging this, Monaco and his colleague Dr. Manuel Vindiola, of the lab's Computational Sciences Division, demonstrated how brain-like computers lend a speedup to the currently best known algorithms for factoring integers.

The team of researchers have devised a way to factor large composite integers by harnessing the massive parallelism of novel computer architectures that mimic the functioning of the mammalian brain. So called [neuromorphic computers](#) operate under vastly different principles than conventional computers, such as laptops and mobile devices, all based on an architecture described by John von Neumann in 1945.

In the von Neumann architecture, memory is separate from the central processing unit, or CPU, which must read and write to memory over a bus. This bus has a limited bandwidth, and much of the time, the CPU is waiting to access memory, often referred to as the von Neumann bottleneck.

Neuromorphic computers, on the other hand, do not suffer from a von Neumann bottleneck. There is no CPU, memory, or bus. Instead, they incorporate many individual computation units, much like neurons in the brain.

These units are connected by physical or simulated pathways for passing data around, analogous to synaptic connections between neurons. Many neuromorphic devices operate based on the physical response properties of the underlying material, such as graphene lasers or magnetic tunnel junctions. Because of this, these devices consume orders of magnitude less energy than their von Neumann counterparts and can operate on a molecular time scale. As such, any algorithm capable of running on these devices stands to benefit from their capabilities.

The speedup acquired by the ARL researchers is due to the formulation of a method for integer factorization with the help of a neuromorphic co-processor. The current fastest algorithms for factoring integers consist primarily of two stages, sieving and a matrix reduction, and the sieving stage comprises most of the computational effort.

Sieving involves searching for many integers that satisfy a certain property called B-smooth, integers that don't contain a prime factor greater than B. Monaco and Vindiola were able to construct a neural network that discovers B-smooth numbers quicker and with greater accuracy than on a von Neumann architecture. Their algorithm leverages the massive parallelism of brain-inspired computers and the innate ability of individual neurons to perform arithmetic operations, such as addition. As neuromorphic architectures continue to increase in size and speed, not limited by Moore's Law, their ability to tackle larger integer factorization problems also grows. In their work, it's estimated that 1024-bit keys could be broken in about a year, a task once thought to be out of reach. For comparison, the current record, a 232 decimal digit number (RSA-768) took about 2,000 years of computing time over the course of several years.

From a broader perspective, this discovery pushes us to question how a shift in computing paradigm might affect some of our most basic security assumptions. As emerging devices shift to incorporate massive parallelism and harness material physics to compute, the computational hardness underlying some security protocols may be challenged in ways not previously imagined. This work also opens the door to new research areas of emerging computer architectures, in terms of

algorithm design and function representation, alongside low-power machine learning and artificial intelligence applications.

"Encrypted messages in warfare often have an expiration date, when their contents become un-actionable," Monaco said. "There is an urgency to decrypt enemy communications, especially those at the field level, since these expire the quickest, compared to communication at higher echelons. In field conditions, power and connectivity are extremely limited. This is a strong motivating factor for using a brain-inspired computer for such a task where conventional computers are not practical."

[18]

## Teaching computers to guide science: Machine learning method sees forests and trees

While it may be the era of supercomputers and "big data," without smart methods to mine all that data, it's only so much digital detritus. Now researchers at the Department of Energy's Lawrence Berkeley National Laboratory (Berkeley Lab) and UC Berkeley have come up with a novel machine learning method that enables scientists to derive insights from systems of previously intractable complexity in record time.

In a paper published recently in the *Proceedings of the National Academy of Sciences (PNAS)*, the researchers describe a technique called "iterative Random Forests," which they say could have a transformative effect on any area of science or engineering with complex systems, including biology, precision medicine, materials science, environmental science, and manufacturing, to name a few.

"Take a human cell, for example. There are  $10^{170}$  possible molecular interactions in a single cell. That creates considerable computing challenges in searching for relationships," said Ben Brown, head of Berkeley Lab's Molecular Ecosystems Biology Department. "Our method enables the identification of interactions of high order at the same computational cost as main effects - even when those interactions are local with weak marginal effects."

Brown and Bin Yu of UC Berkeley are lead senior authors of "Iterative Random Forests to Discover Predictive and Stable High-Order Interactions." The co-first authors are Sumanta Basu (formerly a joint postdoc of Brown and Yu and now an assistant professor at Cornell University) and Karl Kumbier (a Ph.D. student of Yu in the UC Berkeley Statistics Department). The paper is the culmination of three years of work that the authors believe will transform the way science is done. "With our method we can gain radically richer information than we've ever been able to gain from a learning machine," Brown said.

The needs of machine learning in science are different from that of industry, where machine learning has been used for things like playing chess, making self-driving cars, and predicting the stock market.

"The machine learning developed by industry is great if you want to do high-frequency trading on the [stock market](#)," Brown said. "You don't care why you're able to predict the stock will go up or down. You just want to know that you can make the predictions."

But in science, questions surrounding why a process behaves in certain ways are critical. Understanding "why" allows scientists to model or even engineer processes to improve or attain a desired outcome. As a result, machine learning for science needs to peer inside the black box and understand why and how computers reached the conclusions they reached. A long-term goal is to use this kind of information to model or engineer systems to obtain desired outcomes.

In highly complex systems - whether it's a single cell, the human body, or even an entire ecosystem - there are a large number of variables interacting in nonlinear ways. That makes it difficult if not impossible to build a model that can determine cause and effect. "Unfortunately, in biology, you come across interactions of order 30, 40, 60 all the time," Brown said. "It's completely intractable with traditional approaches to statistical learning."

The method developed by the team led by Brown and Yu, iterative Random Forests (iRF), builds on an algorithm called random forests, a popular and effective predictive modeling tool, translating the internal states of the black box learner into a human-interpretable form. Their approach allows researchers to search for complex interactions by decoupling the order, or size, of interactions from the computational cost of identification.

"There is no difference in the computational cost of detecting an interaction of order 30 versus an interaction of order two," Brown said. "And that's a sea change."

In the PNAS paper, the scientists demonstrated their method on two genomics problems, the role of gene enhancers in the fruit fly embryo and alternative splicing in a human-derived cell line. In both cases, using iRF confirmed previous findings while also uncovering previously unidentified higher-order interactions for follow-up study.

Brown said they're now using their method for designing phased array laser systems and optimizing sustainable agriculture systems.

"We believe this is a different paradigm for doing science," said Yu, a professor in the departments of Statistics and Electrical Engineering & Computer Science at UC Berkeley. "We do prediction, but we introduce stability on top of prediction in iRF to more reliably learn the underlying structure in the predictors."

"This enables us to learn how to engineer systems for goal-oriented optimization and more accurately targeted simulations and follow-up experiments," Brown added.

In a [PNAS commentary](#) on the technique, Danielle Denisko and Michael Hoffman of the University of Toronto wrote: "iRF holds much promise as a new and effective way of detecting interactions in a variety of settings, and its use will help us ensure no branch or leaf is ever left unturned." [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  $\text{Na(6)[Mo(12)Ce(6)O(366)H(12)(H(2)O)(78)] \cdot 200 H(2)O}$ , 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 fault-tolerant 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.



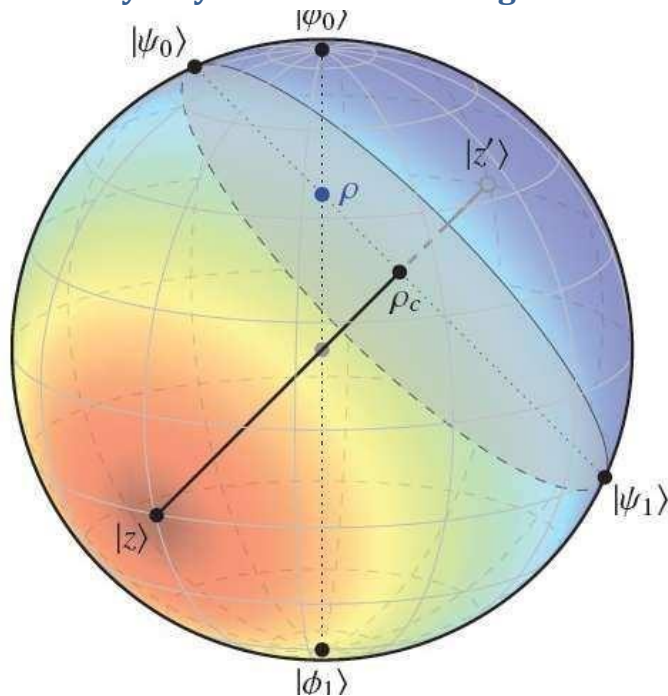
In 2011 Steinberg and his colleagues showed that they could follow trajectories for photons by subjecting many identical particles to measurements so weak that the particles were barely disturbed, and then averaging out the information. This method showed trajectories that looked similar to classical 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  $\rho$  and its radial state  $\rho_c$ . 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.

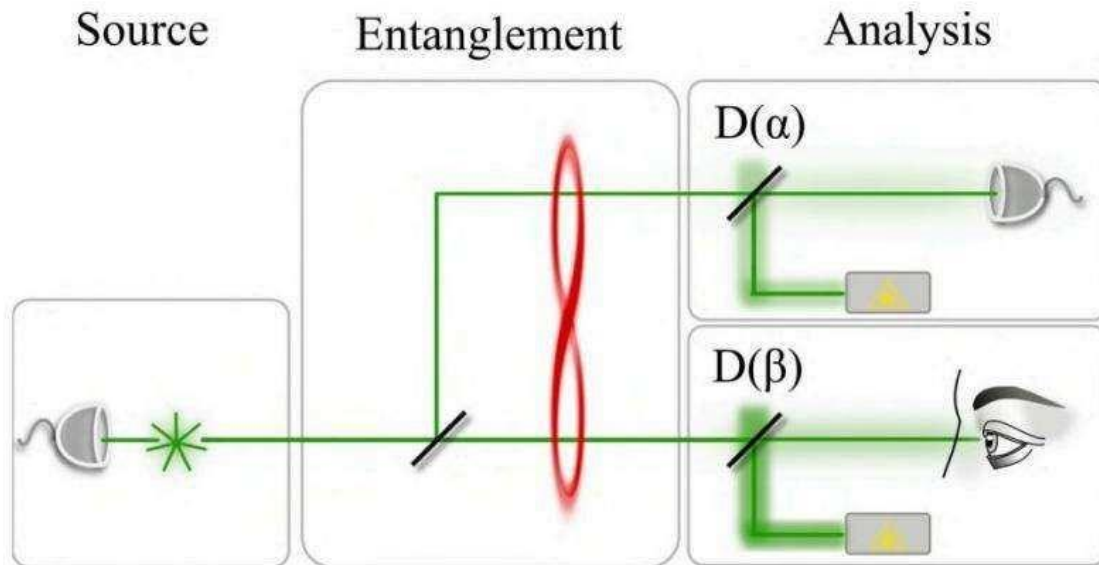
As the scientists explain, the traditionally difficult part of the math problem is that it requires finding the optimal decomposition of mixed states into pure states. The geometrical approach completely eliminates this requirement by reducing the many possible ways that states could decompose down to 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 ever 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 beams 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 its 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 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  $1/2$  spin creator particle to make equal the spins of the weak interaction, for example neutron decay to 2 fermions, every particle is fermions with  $1/2$  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  $1/2$  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 than 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  $\nu$  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  $m_0$  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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