Symposium Artificial Intelligence for Science, Industry and Society

Sunday 20 October 2019 - Friday 25 October 2019

Book of Abstracts

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A machine learning approach for the feature extraction of pulmonary nodules

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In recent times, computational studies have emerged as a viable alternative for complementing the efforts of experienced radiologists in disease diagnosis. Computed tomography (CT) studies are a common way of predicting the lung nodule malignancy for the early diagnosis and treatment of lung cancer in patients. Early detection of the type of nodule is the key to determining the appropriate treatment, thus increasing patient survival. Feature extraction is an important stage in classifying benign and malignant nodules in chest CT scans. However, determining the type of nodule in CT scans is a challenge in medical imaging, since CT images cannot be evaluated as an average or generic image. Hence, the study was based on the application of machine learning techniques, for the feature extraction of pulmonary nodules on a public, Lung TIME dataset, which features scans of teenage and adult patients.

Submitted contributions / 52

AI Applications In Oil Extraction, Review and Case of Study: Convolutional Neural Networks Applied to Seismic Image Analysis

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Application of AI methods in the energy industry has been increasing in the last years. The introduction of AI in the different segments of the energy industry has turned out to be revolutionary. Some of these segments are considered as fundamental for the economic development of countries. This means, increasing their efficiency can highlight the difference between conservatory and vanguardist economies. The ability of AI methods to find patterns in data makes AI a strong tool in decision making. In the energy sector, some of the decisions that must be taken has shown a high level of complexity due to the quantity of features and data that needs to be considered. In such cases, the decisions that are taken by hand, have the risk not be optimum and that the economic waste of the implementation be too high. That is why methods in Deep Learning (DL) and Machine Learning (ML) are being introduced in the decision making process and energetic analysis in different parts of the world. These methods can be applied, for instance, in the prediction of the projections in the different energy markets, the analysis of geophysical data in order to maximize the natural resources and the optimization of the logistic in the energy exploitation, among others. In this work, we want to present a review of some AI methods in the oil industry, and an application example. In this study case, we analyze seismic images applying convolutional neural networks (CNN) to them in order to localize and segment salt bodies, which are of great importance while we are analyzing oil yields. We acknowledge funding from the European Union's Horizon 2020 Programme under the ENERXICO Project, grant agreement No. 828947 and under the Mexican CONACYT-SENER-Hidrocarburos grant agreement No. B-S-69926.

Plenary / **9**

AI Innovation in the Pharmaceutical Sector - Accelerating Research

Plenary / **61**

AI Research at Atos

Author: Cédric Bourrasset[1]

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This lecture will cover the AI research challenges currently addressed by Atos research teams over different domains like Cyber Security, Predictive Maintenance of IT and Privacy by Design needs for Video Intelligence solution in the context current European regulations.

Plenary / **24**

Advances in classification/regression in high energy physics

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Plenary / **17**

Amazon Web Services AI - Deep learning at scale

Author: Nathalie Rauschmayr[1]

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Deep learning is driving rapid progress in fields such as computer vision, natural language processing, and speech recognition. It has become one of the most disruptive technologies and nowadays many products feature artificial intelligence. However, creating production-ready deep learning models involves many challenges: starting from generating good high-quality training datasets to distributed model training, hyperparameter tuning, large scale deployment and many more.

This talk will give an overview of how to build, train, deploy deep learning models on AWS.

Submitted contributions / **51**

An assessment of an ConvNet Applied to Classify Animals in the Wild

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The objective of this work is to show an analysis of the performance of a very well known Convolutional Neural Network applied to the classification of animals in the wild.
The interesting aspect of this application is that the set of images used have diverse characteristics from the training set of the ConvNet.
The analysis goes beyond the typical display of error rates, precision and recall, by being focused on describing situations where the behaviour of the ConvNet is more erratic than expected. For instance, whereas in some cases a misclassification can be explained by a lack of visual information or by the presence of confusing information, we show errors in situations where a correct classification is easily made by a human being.
The aim is to contribute to the discussion of whether current Artificial Neural Networks technologies are suitable to be used in applications with very open and noisy domains.

Submitted contributions / 48

Arhuaco: Deep Learning and Isolation Based Intrusion Detection in High Energy Physics

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High Energy Physics utilizes powerful distributed computational networks called grids, to process and analyze scientific data. Monitoring the security of these networks is a challenging task. Arbitrary and not-trusted applications can be executed inside the grid worker nodes by the scientists. Innovative methods and tools are required to reduce the risk associated with the
execution of users' software (also called jobs), to identify cyber-security incidents and to perform autonomous responses. The isolation and monitoring of job payload activity are necessary in order to protect the computational infrastructure and to find evidence of malicious behavior. We describe a security architecture that integrates Linux containers to safely execute grid jobs with behavior monitoring powered by deep learning methods for the analysis of real-time data to detect and prevent intrusions. A generative method with recurrent neural networks is utilized to improve the detection performance. We describe how these methods aim to increase the security of computational grids, improving existing solutions. We present Arhuaco, a proof-of-concept implementation and provide an evaluation for the ALICE collaboration grid at CERN.

Submitted contributions / 40

Artificial Intelligence and Machine Learnig for Human Mobility in Megacities

Author: Jose L. Mateos[1]

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Human mobility in megacities is a fundamental problem to address and one of the most pressing societal challenges nowadays. Fortunately, we have now at our disposal a vast set of data, through

mobile devices and geolocalized social networks, that allow us to explore, using Data Science, the patterns of mobility of tens of millions of people on a daily basis. We present here recent result for 415 cities in 77 countries using a big data set of the social network Foursquare. Mining this data set we obtained patterns of visitation of attractive sites in megacities that work as a proxy for mobility. We explore these patterns using Artificial Intelligence and Machine Learning to classify and predict statistically mobility patterns according to socio-economic and cultural variations in hundreds of cities around the world.

Plenary / **64**

Atos Quantum Computing: Future Proofing What Lies Beyond Super-Computing

Author: Scott Hamilton[1]

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Organization / **3**

Best poster talks

Organization / **6**

Closing remarks

Authors: Guy Paic[1] ; Lukas Nellen[1]

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Social events / **73**

Conference dinner

The dinner will be held on Thursday, October 24, at the Antigua Hacienda de Tlalpan (http://www.aht.mx/). We will provide transport for the non-local participants from the meeting venue to the restaurant and from the restaurant to the hotels.

The busses will leave the conference venue at 19:00.

Plenary / **23**

Deep Learning for Cosmic-Ray Observatories

Authors: Alexander Temme[1] ; Jonas Glombitza[1] ; Katharina Hafner[1] ; Martin Erdmann[2]

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Ultra-high energy cosmic rays (UHECRs) are the most energetic particles found in nature and originate from extragalactic sources. These particles induce extensive air showers when propagating within the Earth's atmosphere. Cosmic-ray bservatories like the Pierre Auger Observatory measure such air showers using large arrays of surface-detector stations and luorescence telescopes. The reconstruction of event-by-event information sensitive to the cosmic-ray mass is a challenging task and so far, mainly based on the shower shape as measured by fluorescence detector observations with their duty cycle of about 15%.

Recently, significant progress has been made in multiple fields of machine learning using deep neural networks and associated techniques. Applying these new techniques to cosmic-ray physics opens up possibilities for improved reconstructions, including an event-by-event estimation of the cosmic-ray mass using the surface-detector exclusively, exploiting the 100% duty cycle.

In this contribution, we present deep learning-based algorithms applied in the context of cosmic-ray physics. Beside supervised learning for event reconstruction, we investigate methods for understanding the decisions of deep networks which are trained on physics-related tasks. Finally, we discuss strategies for reducing differences between data and physics simulations using adversarial frameworks.

Plenary / **19**

Deep Learning for QCD phase transition and nuclear structure

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Plenary / **71**

Deep learning for cosmology

Author: Celia Escamilla-Rivera[1]

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In this talk I will describe ongoing efforts to shed light on still-unanswered questions in fundamental physics using cosmological observations. I will explain how we can use measurements of the Supernovae data, Baryon Acoustic Oscillations, Cosmic Microwave Background and the large-scale structure of the universe to reconstruct the detailed physics of the dark universe. Also I will address this inverse-problem reconstruction from a Bayesian and Machine Learning perspectives.

Plenary / **22**

Exploring Space in Cyberspace: How Computing and Big Data are Transforming Astronomy

Submitted contributions / 55

From GigScience to Combined Intelligence of Machine and Crowd

Author: Andrey Ustyuzhanin[1]

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Online education captures all new frontiers. Modern platforms are scaled to transfer the necessary information to the student: illustrations of basic concepts, theoretical foundations, etc. At the same time, practical skills are difficult to convey online; they can only be acquired through personal experience. Such difficulties make it difficult to study natural sciences (physics, chemistry, biology, etc.). At the same time, there is a lack of qualification in working with advanced data analysis techniques for solving problems of signal cleaning from noise, optimization of structures, searching for protein structures and hundreds of other tasks. It is seen that, on the one hand, there is an excess of the workforce, of interest in acquiring practice, on the other - a lack of intellectual resources.
This situation leads to an exciting technological win-win project. A possible approach to resolving the contradiction is the creation of a platform to support focal research gig-research teams to work in a competitive-collaborative format. Such working groups consisting of subject matter researchers and online program students will solve both problems: scaling up practical online programs and increasing the level of data analysis technologies used in applied scientific challenges. The story about such a platform is accompanied by a description of examples of practical projects and diverse tasks: from the rules of gamification to the next generation autoML, in the solution of which you can also participate.

Submitted contributions / 44

Galaxy Morphology classification using CNN

Author: Jose Antonio Vazquez-Mata[1]

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Galaxy morphology is one of the most important parameters to understand the assembly and evolution of galaxies in the universe. The most used classification nowadays was proposed by Hubble (1926). This classification is based on the present of disks-, arms-, bulges-like structures, and is carried out mostly by eye identification. Thanks to the upcoming large telescopes and surveys, the new catalogues will contain millions of galaxies, making impossible to carry out a visual classification. Then, convolutional neural networks (CNN) start to play an important role to classify them. In this presentation I sumarise the most recent results (including ours) using machine learning techniques to classify galaxies and future projects.

Submitted contributions / 8

Generative Adversarial Networks for fast simulation: generalisation and distributed training in HPC

Authors: Sofia Vallecorsa[1] ; Federico Carminati[1] ; Gul Rukh Khattak[2]

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Deep Learning techniques have are being studied for different applications by the HEP community: in this talk, we discuss the case of detector simulation. The need for simulated events, expected in the future for LHC experiments and their High Luminosity upgrades, is increasing dramatically and requires new fast simulation solutions. We will describe an R&D activity within CERN openlab, aimed at providing a configurable tool capable of training a neural network to reproduce the detector response and replace standard Monte Carlo simulation. This represents a generic approach in the sense that such a network could be designed and trained to simulate any kind of detector in just a small fraction of time. We will present the first application of three-dimensional convolutional Generative Adversarial Networks to the simulation of high granularity electromagnetic calorimeters. We will describe detailed validation studies comparing our results to Geant4 Monte Carlo simulation, showing, in particular, the very good agreement we obtain for high level physics quantities (such as energy shower shapes) and detailed calorimeter response (single cell response). Finally we will show how this tool can easily be generalized to describe a larger class of calorimeters, opening the way to a generic machine learning based fast simulation approach. To achieve generalization we will leverage advanced optimization algorithms (using Bayesian and/or Genetic approach) and apply state of the art data parallel strategies to distribute the training process across multiple nodes in HPC and Cloud environment. Performance of the parallelization of GAN training on HPC clusters will also be discussed in details.

Plenary / **60**

HPC / AI convergence and computing architecture impacts

Author: Cédric Bourrasset[1]

[1] *Atos*

Science and numerical applications are evolving towards integrating Machine Learning based algorithms. This talk will review future impacts on upcoming HPC architectures.

Plenary / **25**

HPC and AI

Plenary / **65**

Huawei - Introduction to LATAM Intelligent Computing Business and CERN Case Study

Authors: Christian Eduardo Hernandez Garcia[1] ; Su Quing[1]

[1] *Huawei*

Plenary / **69**

IBM Quantum Computing

Author: Panagiotis Barkoutsos[1]

[1] *IBM Zurich*

Plenary / **68**

IBM quantum computing

Author: Vanessa Hernandez[1]

[1] *IBM*

OECD / **70**

Introductory remarks, Mexico

Author: Judith Arrieta[1]

[1] *Minister of the Foreign Service at the Chief of Staff's Office of the Secretary of Foreign Affairs of Mexico*

OECD / **72**

Introductory remarks, OECD

Author: Alan Paic[1]

[1] *OECD*

Submitted contributions / **56**

Large-Scale Scientific endeavours: the production and dissemination of advance computer science's knowledge

Author: Arturo Sanchez Pineda[1]

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Perform big data analysis and visualisation on your own computer? Yes, you can! Commodity computers are now very powerful in comparison to only a few years ago. On top of that, the performance of today's software and data development techniques facilitates complex computation with fewer resources. Cloud computing is not always the solution, and reliability or even privacy is regularly a concern. While the Infrastructure as a Service (IaaS) and Software as a Service (SaaS) philosophies

are a key part of current scientific endeavours, there is a misleading feeling that we need to have remote computers to do any kind of data analysis. One of the aims of the ATLAS Open Data project is to provide resources — data, software and documents — that can be stored and executed in computers with minimal or non-internet access, and in as many different operating systems as possible. This approach is viewed as complementary to the IaaS/SaaS approach, where local university, students and trainers' resources can be used in an effective and reproducible way — making the HEP and Computer Sciences fields accessible to more people. We present the latest developments in the production and use of local Virtual Machines and Docker Containers for the development of physics data analysis. We also discuss example software and Jupyter notebooks, which are in constant development for use in classrooms, and students' and teachers' computers around the world. Finally, we showcase how those tools are developed and in use by international efforts (IPPOG, ICTP-PWF and CEVALE2VE.org) in Latin America and Europe to bring knowledge in countries like Mexico, Venezuela, Colombia, Peru, Ecuador, Argentina and Uruguay with support of the ICTP, CERN and many universities in the region.

Plenary / **13**

Leveraging AI Communities as Innovation Engines in Life Sciences

The generation of large-scale biomedical data is creating unprecedented opportunities for applications of AI solutions. Typically, the data producers develop initial predictions using AI, but it is very likely that the higher performing AI methods may reside with other groups. Crowdsourcing the analysis of complex and massive data has emerged as a framework to find robust methodologies in healthcare and drug discovery. When the crowdsourcing is done in the form of collaborative scientific competitions, known as Challenges, the validation of the AI methods is inherently addressed. Challenges also encourage open innovation, create collaborative communities to solve diverse and important biomedical problems, and foster the creation and dissemination of well-curated data repositories.

Submitted contributions / **31**

Machine Ethics Frameworks and Practical Implications for AI & DS

Author: Jesus Ramos[1]

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Talk given at SXSW 2019 in Austin, TX.
Contrary to what tech news outlets like Mashable, Techcrunch, and Wired tell us about the future of work and the purported "rise of the machines", we're seeing that Machine Learning developments are still far away from general AI, and hence far away from becoming real problem solvers. However, it is precisely because of this early stage of development that engineers and mathematicians need to talk about the real, down-to-earth implications of imbuing their algorithms and models with ethical considerations. We will discuss these, specifically for supervised, unsupervised and reinforcement learning, and will share some flops and bloopers from both sides of the border. We will then finish this talk with 3 frameworks for ethical modelling.

Plenary / **10**

Machine Learning in High Energy Physics

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Plenary / **26**

Machine Learning in High Energy Physics

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Submitted contributions / **57**

Machine Learning in Velo LHCb monitoring and calibration in Run I and II.

Author: Maciej Witold Majewski[1]

[1] *AGH University of Science and Technology (PL)*

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Studies of High energy physics rely on cutting edge technology of particle detectors. These detectors are working under harsh conditions of constant radiations, and their operation must be strictly supervised to achieve maximum efficiency and quality of data taking. The LHCb's Vertex Locator is a strip silicon detector used in Run I and II of Large Hadron Collider. We study the application of machine learning algorithms for some of the monitoring and maintenance tasks. In this work, we present solutions based on data taken during Run I and II, that should inspire similar methods for new VeloPix detector in run III in 2021.

Submitted contributions / **28**

Machine Learning-Based System for the Availability and Reliability Assessment and Management of Critical Infrastructures

Author: Luigi Serio[1]

Co-authors: Ugo Gentile [1] ; Federico Antonello [2] ; Piero Baraldi [2] ; Enrico Zio [2]

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A critical infrastructure is a complex interconnected system of systems providing basic and essential services to support the operation of particle accelerators but also industries and households for which they must guarantee high reliability of critical functions.
Model-based approaches are usually adopted to provide an early identification of failures and to reveal hidden dependencies among subsystems. System models are complex and require constant

updating to be reactive to system changes and real operating conditions, wear and aging. The interconnections between the different systems and the functional dependencies between their components are in many cases modified at both physical and functional levels while their degraded performances impact the overall system availability and reliability.
A novel approach is proposed which combines model-based and Big Data analytics by machine learning techniques to extract descriptive and predictive models directly from data. The objective is to foresee and react in time to failures to reduce downtimes as well as to optimize maintenance and operation costs.
The Computer-Aided System for critical infrastructure Operation (CASO) is designed to significantly and efficiently enhance the quality, safety, reliability and availability of critical infrastructures.
We report on the design of CASO, its implementation and on the preliminary results inferred on historical and live stream data recorded from CERN's technical infrastructure. Proposal for the full deployment and expected long-term capabilities will also be discussed.

Plenary / **18**

Machine learning for neutrino identification

Author: Saul Alonso Monsalve[1]

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This talk will cover the current state of machine learning (ML) in neutrino experiments. In experiments like the Deep Underground Neutrino Experiment (DUNE), NuMI Off-axis νe Appearance (NOvA), the Micro Booster Neutrino Experiment (MicroBooNE), and Argon Neutrino Teststand (ArgoNeuT), deep learning (DL) approaches based around convolutional neural networks have been developed to provide highly accurate and efficient selections of neutrino interactions. Moreover, there is also other exciting ongoing work in DUNE focused on applying ML to tasks such as developing Generative Adversarial Networks (GANs) for photon simulation; or using Graph Neural Networks for track vs. shower hit-classification. In addition to the above, DUNE is also collaborating with high-tech companies to run some of their ML models on Tensor Processing Unit (TPU), and Field-programmable gate array (FPGA), specific hardware provided by Google and Micron Technology, respectively. Finally, the Tokai to Kamioka (T2K) experiment is also using a novel DL approach for the 3D reconstruction of the SuperFGD detector events.

Plenary / **58**

Machine learning in accelerator physics: applications at the CERN Large Hadron Collider

Authors: Belen Maria Salvachua Ferrando[1] ; Elena Fol[2] ; Fred Blanc[3] ; Frederik Van Der Veken[4] ; Gabriella Azzopardi[4] ; Gianluca Valentino[4] ; Loic Thomas Davies Coyle[3] ; Massimo Giovannozzi[1] ; Michael Schenk[3] ; Rogelio Tomas Garcia[1] ; Stefano Redaelli[1] ; Tatiana Pieloni[5]

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With the advent of machine learning a few decades ago, Science and Engineering have had new powerful tools at their disposal. Particularly in the domain of particle physics, machine learning

techniques have become an essential part in the analysis of data from particle collisions. Accelerator physics, however, only recently discovered the possibilities of using these tools to improve its analysis. In different laboratories worldwide, several activities are being carried out, typically in view of providing new insights to beam dynamics in circular accelerators. This is, for instance, the case for the CERN Large Hadron Collider, where since a few years exploratory studies are being carried out, covering a broad range of topics. These include the optimisation of the collimation system, the anomaly detection of beam position monitors, analysis of optimal correction tools for linear optics, lifetime and performance optimisation, and detection of hidden correlations in the huge data set of beam dynamics observables collected during the LHC Run 2. Furthermore, very recently, machine learning techniques are being scrutinised for the advanced analysis of numerical simulations data, in view of improving our models of dynamic aperture evolution.

Submitted contributions / 47

Network science to analyse insecurity perturbations that undermine Mexican tourism industry

Authors: Tanya Arenas[1] ; Tanya Arenas[2]

Co-authors: Felipe Lara [3] ; Valentín Jiménez [4] ; Miguel A. Martínez

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[4] *Tecnológico de Estudios Superiores del Oriente del Estado de México*

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The increasing availability of data due to effective and fast sharing methods offered by technological advances has catalyzed new approaches like network science to process large data sets and transcend traditional statistical tools analysis; hence we introduce the tripartite: destinations-rates-advisories network to make connections between complex non-linear interrelations that affect Mexican tourism industry. In the construction of this network the first set of nodes are 70 main Mexican tourist destinations; the second set corresponds to occupancy rates each destination had in 2017 and 2018; and the third set captures travel advisories emitted in 2017 and 2018 for some Mexican tourist destinations. Our network analysis is an attempt to extract useful information from a large amount of data, identifying occupancy rates prevalence, variation and their correlation with travel advisories; pertinent to develop deep understanding of tourism encoded interactions and to lead informed strategic decision making and operational coordination to amplify range of responses to adverse scenarios in tourism industry.

Organization / 66

Neural Network optimisation

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Modern neural network architecture reflects the complexity of the problem. So those may become quite complex and computationally heavy. Usually, there are plenty of different meta-parameters to tune: number of layers, activation function, number of neurons per layer, drop-out rate, etc. There many different methods and tools that aimed at tuning those parameters for various reasons - accuracy, memory footprint or inference rate. This mini-course will cover the basics approaches for neural networks optimizing including hyperparameter optimization, network architecture search and Bayesian Neural Network perspective. Practical hands-on sessions will follow the theoretical introduction.

Organization / **4**

OECD summary

Author: Alan Paic[1]

[1] *OECD*

Submitted contributions / **54**

Online Estimation of Particle Track Parameters based on Neural Networks for the Belle II Trigger System

Authors: Kai Lukas Unger[1] ; Steffen Baehr[2]

Co-authors: Christian Kiesling [3] ; Felix Meggendorfer [4] ; Juergen Becker [2] ; Sara McCarney ; Sebastian Skambraks [5]

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The Belle II particle accelerator experiment is experiencing substantial background from outside of the interaction point. To avoid taking data representing this background, track parameters are estimated within the pipelined and dead time-free level 1 trigger system of the experiment and used to suppress such events. The estimation of a particle track's origin with respect to the z-Axis, which is along the beamline, is performed by the neural z-Vertex trigger. This system is estimating the origin or z-Vertex using a trained multilayer perceptron, leveraging the advantages of training to current circumstances of operation. In order fulfil the requirements set by the overall trigger system it has to provide the estimation within an overall latency of 5 µs while matching a refresh rate of up to 31.75 MHz for new track estimations. The focus of this contribution is this system's current status. For this both implementation and integration into the level 1 trigger will be presented, supported by first data taken during operation as well as figures of merit such as latency and resource consumption. In addition its upgrade plan for the near future will be presented. The center of these is a Hough based track finding approach that uses Bayes theorem for training the weighting of track candidates. Characteristics of this system's current prototypical implementation on FPGAs as well as present plants towards integration for future operation will be presented.

OECD / **30**

Panel discussion

Panel members (speakers):

- Julien Chiaroni from General Secretariat for Investment (Office of the Prime Minister, France) - developing "trustable" AI.
- Mirjana Stankovic, Vice-President, Emerging Technologies at Tambourine ventures - what can be done when policies develop more slowly than technology?

- Ashley Casovan, Executive Director of AI Global, a non-profit dedicated to responsible implementation of AI will talk about responsibility and ethics with AI, as well as future certification of AI technologies.
- Cédric Bourrasset, Artificial Intelligence product manager at ATOS will speak about ethical choices in videosurveillance applications
- Prof. Andrea Bertolini, Dirpolis Institute and University of Pisa will speak about regulation in AI and robotics
- Yan Zhenfang, General Director of Intelligent Computing Dept. of Huawei will speak about the experience of Huawei
- Andrea Escobedo Lastiri, IBM, will talk about policy issues and AI ethics as practiced by IBM

OECD / **29**

Panel discussion

Panel members (speakers):

- Andreas Hartl, Head of Division on Artificial Intelligence and Data Economy, German Ministry of Economy - responsible for the implementation of the German AI strategy, and drafting a Blockchain strategy.
- Ana Valcarel Orti, INRIA and Project Manager, Co-ordination of the French national plan of research in AI
- Cristina Martínez Pinto, AI for Good Lab Director at CMINDS (NGO) - a future AI strategy in Mexico
- Estelle Parker, Australian Embassy in Mexico - AI ethics in Australia
- Ashley Casovan, Executive Director of AI Global, formerly Director of Data Architecture and Innovation at the Government of Canada - Canadian AI strategy

Submitted contributions / **7**

Perspectives of Deep learning techniques in Lattice 1+1d Scalar Field Theory

Author: Kai Zhou[1]

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We explore the perspectives of machine learning techniques in the context of quantum field theories based on our recent publication[1]. In particular, we discuss two-dimensional complex scalar field theory at nonzero temperature and chemical potential – a theory with a nontrivial phase diagram.

A neural network is successfully trained to recognize the different phases of this system and to predict the value of various observables, based on the field configurations. We analyze a broad range of chemical potentials and find that the network is robust and able to recognize patterns far away from the point where it was trained. Aside from the regressive analysis, which belongs to supervised learning, an unsupervised generative network is proposed to produce new quantum field configurations that follow a specific distribution. An implicit local constraint fulfilled by the physical configurations was found to be automatically captured by our generative model. We elaborate on potential uses of such a generative approach for sampling outside the training region.

[1] Phys.Rev. D (R)100 (2019) no.1, 011501

Submitted contributions / 45

Portraying Double Higgs at the Large Hadron Collider

Authors: Jeong Han Kim[1] ; K.C. Kong[1] ; Konstantin Matchev[2] ; Minho Kim[3] ; Myeonghun Park[4]

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We examine the discovery potential for double Higgs production at the high luminosity LHC in the final state with two b-tagged jets, two leptons and missing transverse momentum. Although this dilepton final state has been considered a difficult channel due to the large backgrounds, we argue that it is possible to obtain sizable signal significance, by adopting a deep learning framework making full use of the relevant kinematics along with the jet images from the Higgs decay. For the relevant number of signal events we obtain a sub- stantial increase in signal sensitivity over existing analyses. We discuss relative improvements at each stage and the correlations among the different input variables for the neutral network. The proposed method can be easily generalized to the semi-leptonic channel of double Higgs production, as well as to other processes with similar final states.

Submitted contributions / 35

Randomness Characterization through Bayesian Model Selection

Authors: Rafael Diaz Hernandez Rojas[1] ; Aldo Solís[2] ; Alí Angulo Martínez[2] ; Alfred U'Ren[2] ; Jorge Hirsh[2] ; Matteo Marsili[3] ; Isaac Pérez Castillo[2]

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Random number generation currently plays a fundamental role due to its several applications in probabilistic algorithms (*e.g.* Monte Carlo methods, stochastic gradient descent, etc.), but mainly for its importance in cryptography. The most common methods for characterizing random numbers generators (RNG) either lack formality (*e.g.* the battery of tests provided by the NIST) or are not generally applicable, even in principle (*e.g.* the characterization developed by the Algorithmic

Information Theory). In this work we present a method based on Model Selection using Bayesian Inference which turns out to be both rigorous and effective in assessing the randomness of bits sequences. We are able to obtain analytic expressions for a model's likelihood and our results shows that this new method is more stringent than both the NIST's set of tests and the Borel's Normality criterion. Additionally, given that Bayesian Inference entails the generalizability feature for the selected model, our scheme transcends single sequence analysis and provides a characterization of the *source* acting as a RNG. (More details and and experimental case are presented in Ref. [1].)

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Registration desk open

Submitted contributions / 38

Regularization methods vs large training sets

Authors: Juan Jaime Vega Castro[1] ; Juan Jaime Vega Castro[None]

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Digital pulse shape analysis (DPSA) is becoming an essential tool to extract relevant information from waveforms arising from different source. For instance, in the particle detector field, digital techniques are competing very favorable against the traditional analog way to extract the information contained in the pulses coming from particle detectors. Nevertheless, the extraction of the information contained in these digitized pulses requires powerful methods. One can visualize this extracting procedure as a pattern recognition problem. To approach this problem one can use different alternatives. One very popular alternative is to use an artificial neural network (ANN) as a pattern identifier. When using an ANN, it is common to introduce a regularization method in order to get rid or at least to reduce the effects of overfitting and overtraining. In addition, another option that helps to solve these problems is to use a large training dataset to train the ANN. In this paper, we make an intercomparison of the advantage of regularization methods vs large training datasets when used as methods to reduce the overtraining and overfitting effects when training an ANN.

Plenary / 59

Regulating Emerging Technologies: Opportunities and Challenges for Latin America

Author: Mirjana Stankovic[1]

[1] *Vice President, Emerging Tech and Intellectual Property, Tambourine Innovation Ventures*

"Can regulators keep up with fintech?" "Your Apps Know Where You Were Last Night, and They're Not Keeping It Secret." "Regulators scramble to stay ahead of self-driving cars." "Digital health dilemma: Regulators struggle to keep pace with health care technology innovation." Headlines like these capture a central challenge to today's regulators.

Existing regulatory structures are often slow to adapt to changing social and economic circumstances, and are generally risk-averse. The policy cycle often takes anything from five to 20 years whereas a unicorn startup can develop into a global company in just a few months. Airbnb, for example, went from 21,000 arrivals in 2009 to 80 million in 2016. In the meantime, cities and countries are still trying to figure out how, and if, they can regulate short-term rental markets. Ride-hailing services, such as Uber, have experienced similar hyper-growth as regulations in the space struggle to follow. As new innovation and business models emerge government agencies are challenged with creating, adapting, enforcing and communicating the regulations to the public at a previously undreamed-of pace. And they must do so while working within legacy frameworks and attempting to foster innovation.

This presentation will highlight the unique regulatory challenges posed by digital-age technologies. Then it will describe the four critical questions policymakers and regulators in Latin America must address when it comes to regulating the Fourth Industrial Revolution. Finally, it will provide a set of five principles to guide the future of regulation.

Plenary / **15**

Robotics, AI, and machine vision

In this talk it is presented the semantic-reasoning module of VIRBOT, our proposed architecture for service robots.
We show that by combining symbolic AI with digital-signal processing techniques this module achieves competitive performance.
Our system translates a voice command into an unambiguous representation that helps an inference engine, built around an expert system, to perform action and motion planning.
First, in the natural-language interpretation process, the system generates two outputs: (1) conceptual dependence,
expressing the linguistic meaning of the statement, and (2) verbal confirmation, a paraphrase in natural language that is
repeated to the user to confirm that the command has been correctly understood.
Then, a conceptual-dependency interpreter extracts semantic role structures from the input sentence and looks for such
structures in a set of known interpretation patterns.
We evaluate this approach in a series of skill-specific semantic-reasoning experiments.
Finally, we demonstrate our system in the general-purpose service robot test of the RoboCup-at-Home international competition,where incomplete information is given to a robot and the robot must recognize and request the missing information, and we compare our results with a series of baselines from the competition where our proposal performed best.

Plenary / **62**

Scaling Deep Learning to Exascale – ACM Gordon Bell Prize 2018

Author: Pedro Mario Cruz e Silva[1]

[1] *NVidia*

In this talk I will present technical details about the ACM Gordon Bell Prize winner project at Supercomputing 2018. In this work the joint team from NERSC and NVIDIA succeeded in scaling a Deep Learning training across 27.000+ GPUs in Summit (world's largest HPC system) and obtained a high fraction of peak performance. This research showed that realistic scientific applications could leverage mixed precision with FP16 (without loss of accuracy). A Deep Learning approach to segmenta-

tion of Atmospheric Rivers (AR) and Tropical Cyclones (TC) was applied to achieve state-of-the-art pattern detection for characterizing extreme weather. The training was performed at an impressive performance of peak (sustained) FP16 performance of 1.13 EF/s (1.0 EF/s). To achieve this Exascale breakthrough several innovations were developed both in Software and Hardware. These new technologies in software (TensorFlow, NCCL, etc) and hardware (Volta, Tensor Cores, NVLINK, etc) will be explained during the presentation.

Submitted contributions / **50**

Similarity Hashing and Learning for Tracks Reconstruction

Author: Sabrina Amrouche[1]

Co-authors: Moritz Kiehn [2] ; Andreas Salzburger [3] ; Tobias Golling [2]

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At the High Luminosity Large Hadron Collider (HL-LHC), many
proton-proton collisions happen during a single bunch crossing. This leads on average to tens of thousands of particles emerging from the interaction region. Two major factors impede finding charged particle trajectories from measured hits in the tracking detectors. First, deciding whether a given set of hits was produced by a common particle is an under-specified task. State-of-the-art reconstruction models usually tackle this issue via so-called track following only at a later stage after considering many hits. Second, assuming a nearly perfect hit-particle decision function, constructing possible hit combinations to their compatibility using this decision function is a combinatorial problem. Thus, the traditional approach will grow exponentially as the number of simultaneous collisions increase at the HL-LHC and pose a major computational challenge.

We propose a framework for Similarity Hashing and Learning for Track Reconstruction (SHLTR) where multiple small regions of the detector are reconstructed in parallel with minimal fake rate. We use hashing techniques to separate the detector search space into buckets. The particle purity of these buckets, i.e. how many hits from the same particle are contained, is increased using locality sensitivity in feature space where per-hit features beyond just its position are considered. The bucket size is sufficiently small to significantly reduce the complexity of track reconstruction within the buckets or regions.

A neural network selects valid combinations in the buckets and builds up full trajectories by connected components search independently of global positions of the hits and detector geometry. The whole process occurs simultaneously in the multiple regions of the detector and curved particles are found by allowing buckets to overlap. We present first results of such a track reconstruction chain including efficiency, fake estimates, and computational performances in μ=200 datasets.

Plenary / **14**

Simulating Quantum Computing System with Digital Twins for Accelerated AI

Plenary / **20**

Simulation and generative models in high energy physics

Author: Tobias Golling[1]

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High-energy particle physic experiments rely heavily on billions of CPU hours per year for data processing purposes. The production of synthetic data through Geant4-based Monte Carlo simulation describing particle shower developments in the calorimeter is the single most compute-intensive tasks. Fast simulation techniques are already today indispensable. With the upcoming high-luminosity upgrade of the LHC experiments even larger simulated datasets are needed to support physics analyses. Current "classical" fast calorimeter simulation techniques are based on parametrizations of the calorimeter response. Generative models have the potential to learn the appropriate detector output response. The goal is to replace the slow but accurate Geant4-based Monte Carlo simulation by a fast, generic and accurate (enough) generative model. Both studies of Variational Auto-Encoders (VAEs) and Generative Adversarial Networks (GANs) will be presented.

Submitted contributions / 63

Skin Lesion Detection in Dermatological Images using Deep Learning

Authors: Boris Escalante-Ramírez[1] ; Jimena Olveres[1] ; José Carlos Moreno-Tagle[1]

[1] *UNAM*

We demonstrate that it is possible to approach the skin lesion classification problem as a detection problem (multiple localization with classification), a much more complex and interesting problem with satisfactory and promising results. The image dataset used in the experiments comes from the ISIC Dermoscopic Archive, an open-access dermatology repository. In particular, the ISIC 2017 dataset, a subset of the ISIC archive, released for the annual ISIC challenge was used. We show that it is possible to adapt a high quality imaging dataset to the requirements demanded by a deep learning detection architecture such as YOLOv3 [10]. After the training process is completed, the detector is able to identify and locate three different types of skin lesions in real-time. Finally, we describe some of the next steps we are taking to improve the performance of this proposed solution as we seek to deploy in the near future a real-time deep learning solution in a smartphone app that could be used by a medical specialist as well as the general public.

Submitted contributions / 36

Studying the parton content of the proton with deep learning models

Authors: Juan Manuel Cruz Martínez[1] ; Stefano Carrazza[1]

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Parton Distribution Functions (PDFs) model the parton content of the proton. Of the many collaborations which focus on PDF determination in the last 20 years, NNPDF was pioneer on the use of Neural Networks to model the probability of finding partons (quarks and gluons) inside the proton with a given energy and momentum.

In this work we introduce state of the art techniques to modernize the NNPDF methodology and study different models and architectures in a systematic way which allows as to assess the quality of the PDF fit: overtraining, model complexity, hyperparameter setup, optimization algorithm...

We show a fully automatized pipeline to achieve a best model setup finding good improvements in both the quality and efficiency of the fits.

Organization / **5**

Symposium summary

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Plenary / **67**

The Mode of Computing

Author: Luis Pineda[1]

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The Turing Machine is the paradigmatic case of computing machines, but there are others, such as Artificial Neural Networks, Table Computing, Relational-Indeterminate Computing and diverse forms of analogical computing, each of which based on a particular underlying intuition of the phenomenon of computing. This variety can be captured in terms of system levels, re-interpreting and generalizing Newell's hierarchy, which includes the knowledge level at the top and the symbol level immediately below it. In this re-interpretation the knowledge level consists of human knowledge and the symbol level is generalized into a new level that here is called The Mode of Computing. Natural computing performed by the brains of humans and non-human animals with a developed enough neural system should be understood in terms of a hierarchy of system levels too. By analogy from standard computing machinery there must be a system level above the neural circuitry levels and directly below the knowledge level that is named here The mode of Natural Computing. A central question for Cognition is the characterization of this mode. The Mode of Computing provides a novel perspective on the phenomena of computing, interpreting, the representational and non-representational views of cognition, and consciousness.

Submitted contributions / **46**

The QUA³CK Machine Learning Development Process and the Laboratory for Applied Machine Learning Approaches (LAMA)

Authors: Christopher Meier[1] ; Daniel Grimm[1] ; Gabriela Molinar[1] ; Juergen Becker[1] ; Marco Stang[1] ; Simon Stock[1] ; Tim Hotfilter[1] ; Wilhelm Stork[1]

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According to recent studies, Machine Learning has become a demanded skill in the world of engineering. Therefore, it is possible to find hundreds of online courses offering to teach these abilities. Some companies now call for 'Machine Learning Engineers' as a new hiring position. For many engineering students this is a very difficult situation, since taught courses are often focusing on the theoretical backgrounds of machine learning. However, in order to learn the correct use of machine learning methods, students have to apply them to real world problems. Hence, the scientists of the Institute for Information Processing Technologies (ITIV) at the Karlsruhe Institute of Technology (KIT, Germany) created the Laboratory for Applied Machine Learning Approaches (LAMA). We strive for a wide audience of engineering students, independently of their previous machine learning experience. The students go through three phases of learning. First, they get introduced to the theoretical concepts, then they will undertake guided hands-on experiments and lastly there is a creative 'Into-the-Wild'-part. This approach was very successful and was positively received by the students.
The lab was designed around a novel machine learning process. This methodology is an adaptation of CRISP-DM, which is a unified cross-industry standard. However, it did not find general acceptance in academia. One reason might be the strong emphasis on business understanding.
We developed a simplified and easy-to-remember version of the CRISP-DM. This new machine learning process, which we named QUAAACK or QUA3CK, is an important part of the contribution of this work. It is an acronym for the individual process steps. The method commences with Question and Understanding the data. Followed by the iterative A^3-process: Algorithm selection, data Adaption and parameter Adjustment. Based on these we will Conclude and compare the results and finally do the Knowledge transfer into a solution, product or publication. Figure 1 displays the process with precise description of each individual step.
![Figure 1: The LAMA teaches the iterative QUAAACK process as part of the lab.][1]
The laboratory is composed of two main parts: Guided assignments and the project based 'Into-the-Wild' phase. First, we teach students the basic concepts of frequently used machine-learning algorithms in theory and practice. We are using the widely adapted programming language 'python' for the guided part of the laboratory. Utilizing 'jupyter notebooks' we combine theoretical background documentation and its associated code in an interactive manner.
During the 'Into-the-Wild' part, students have the possibility to apply their learned skills to a real world engineering challenge. The aim of this creative part is to apply the QUA3CK process. Groups of two to four students can seek their own challenge or use provided datasets by the institute. In the end, all teams present their results to the other students and tutors. There was a broad variety of students' projects in summer 2019. Examples were a music composing neural network, the detection of sitting behaviour in order to improve posture and classifying whether bees are affected by toxins. We can conclude that self-imposed goals lead to a better intrinsic motivation and a higher identification with the project.

Plenary / **21**

Towards inverse design in chemistry: from prediction to deep generative models

Author: Benjamin Sanchez-Lengeling[1]

[1] *Google Brain*

Many of the challenges of the 21st century, from personalized healthcare to energy production and storage, share a common theme: materials are part of the solution. Groundbreaking advances are likely to come from unexplored regions of chemical space. A central challenge is, how do we design molecules and materials according to a desired functionality?
In this talk I showcase how we can apply machine learning to a variety of chemical problems centered around two main themes: 1) building data-driven models for prediction and interpretation of molecular properties and 2) generating and optimizing molecules according to properties via deep generative models.

Plenary / **11**

Trustworthy AI - The AI4EU approach

Author: Ulises Cortes[1]

[1] *Barcelona Supercomputing Center*

Plenary / **12**

Upcoming Big Data and AI Challenges in Astronomy

Author: Željko Ivezić[1]

[1] *University of Washington*

Plenary / **27**

Variational Autoencoders for Medical Imaging

Author: Juan Cerrolaza[1]

[1] *Accenture Iberia - Artificial Intelligence Group*

With the advent of deep learning-based techniques, new approaches and novel architectures are proposed every day, improving the state of the art in almost every technical discipline, including medical imaging. Autoencoders are one of the most popular unsupervised deep learning techniques. Thanks to their unsupervised nature, autoencoders, and its several variants, such as variational autoencoders, provide high-capacity, unbiased, multi-dimensional vector representation of information, proving effective in many applications, including feature extraction, diagnosis, and image reconstruction. In this presentation, we will review some of the most recent advances of deep convolutional autoencoders, but always with a special focus on their practical applications in medical imaging, including prenatal and cardiac imaging.

Submitted contributions / **42**

Visual comparison of particle collisions in the TPC in the ALICE Experiment

Author: Wiktor Kozakowski[1]

Co-authors: Lukasz Kamil Graczykowski [1] ; Tomasz Piotr Trzcinski [1]

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The comparison of particle collisions is a key component of an understanding of high-energy physics experiments. It allows the user to check their theoretical knowledge with empirical results. The methods which currently are used mainly focus on properties of collision and collided particles itself. In this work, we present the new solution for this task, using real-life examples from the Time Projection Chamber (TPC) in the ALICE experiment at CERN. It focuses on the visual representation of particles in 3D space instead of properties of particles collision. For this purpose, we used the machine learning model - VAE (Variational Autoencoder). The obtained result we compared with

edge histogram descriptor which is the algorithm used in MPEG-7 Visual Standard to measure the similarity of edges.

The main advantage of the proposed method is finding a similar collision in terms of visual representation. Apart from this, the complexity of these algorithms is linear, the same as it is in traditional methods. Nevertheless, this quality of finding a similar collision comes with the cost of execution time. It is about 4 times slower than the model based on physical properties.

1

Welcome Event

Organization / **16**

Welcome and introduction